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CMB7 User's Manual

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CMB7 User's Manual

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16. ABSTRACT

The Chemical Mass Balance (CMB) receptor model uses chemical composition measured in the source and receptor samples to estimate the relative contributions of different source categories to ambient particulate concentration.

This manual describes the CMB7 receptor model software. It is designed to allow users to use the CMB receptor model constructively with a few hour's learning time. Emphasizing rapid command of modeling procedures, the manual covers primarily the mechanical aspects of operating the model. Information on the theoretical basic principles of CMB receptor modeling is also briefly explained in the appendices of this manual.

This manual is intended for wide use by State and local air pollution control agency personnel in developing State Implementation Plans (SIPs) for PM10. The U. S. Environmental Protection Agency has published a companion document to this manual that should be consulted for this application. The Protocol for Applying and Validating the CMB Model, EPA-450/4-87-010, provides guidance on applicability, assumptions and interpretation of results. This protocol provides a practical strategy for obtaining valid results.

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CMB7 USER'S MANUAL

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ABSTRACT

The Chemical Mass Balance (CMB) receptor model uses chemical concentrations measured in source and receptor samples to estimate the contributions of different source types to ambient pollutant concentrations. The model is used primarily in the development of State Implementation Plans for PM_{10}. CMB7 is a software package which implements the model. This interactive software operates on IBM compatible microcomputers and allows the user to: 1) select samples, chemical species, and source types for modeling; 2) calculate source contributions and their standard errors using the effective variance least squares estimation algorithm; 3) evaluate the goodness of fit and validate the model results; 4) prepare outputs for reports and input to data base and spreadsheet software; and 5) graph results.

The User's Manual describes model installation, the command menu, and the structure of input and output data files. A step-by-step tutorial using example data files, which are included on a floppy disk with the executable computer code, is provided. Sources of ambient and source profile data for PM_{10} are described.

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SECTION 1

INTRODUCTION

The Chemical Mass Balance (CMB) air quality model is one of several receptor models which have been applied to air resources management. Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations. Receptor models are generally contrasted with dispersion models which use estimates of pollutant emissions rates, meteorological transport, and chemical transformation mechanisms to estimate the contribution of each source to receptor concentrations. The two types of models are complementary, with each type having strengths which compensate for the weaknesses of the other. The current guidance for the development of PM_{10} State Implementation Plans (SIPs) recommends the application of both receptor and dispersion models with a reconciliation of their independent source apportionments (U.S. EPA, 1987c).

This software manual updates Volume III of EPA's Receptor Model Technical Series by describing the fundamentals and use of CMB7. Volume III (U.S. EPA, 1987a) describes the earlier CMB 6.0 of the CMB software.

The primary objectives of this manual are:

- To identify the new features and improvements in CMB modeling software.
- To provide instructions in the use of the new software.
- To identify additional examples of CMB applications to PM_{10}, visibility, and gaseous species.

This manual is intended for wide use by state and local air pollution control agency personnel in developing State Implementation Plans for PM_{10} (suspended particulate matter with an aerodynamic diameter less than 10 μm).

The U.S. Environmental Protection Agency (EPA) has published two companion documents to this manual that are also SIP-oriented and that should be consulted for SIP development. The first, "Protocol for Applying and Validating the CMB Model" (U.S. EPA, 1987b), provides guidance on applicability, assumptions, and interpretation of results. The protocol provides a practical strategy for obtaining valid results. The second document, "Protocol For Reconciling Differences Among Receptor and Dispersion Models" (U.S. EPA, 1987c), recommends a procedure for examining and reconciling differences between receptor and dispersion modeling results.

This manual is not intended to describe fully the CMB or other receptor models or their applicability to different situations. Several review articles, books, and conference proceedings provide additional information about the CMB and other receptor models (Hopke and Dattner, 1982; Stevens and Pace, 1984; Hopke, 1985; Pace, 1986; Gordon, 1980, 1988; Watson, 1989).

1.1 WHAT THE MODEL DOES

The CMB model uses the chemical composition of ambient pollution samples to estimate the contributions of different source types to the measured pollutant concentrations. The CMB model has been most widely used for suspended particulate matter, but it is equally applicable to gaseous species. The chemical composition of each source-type's emissions (source profile) must also be known to use the model. The information required by and produced by the CMB model is shown in Figure 1.

The CMB model quantifies contributions from chemically distinct source-types rather than contributions from individual emitters. For example, the model might calculate that 6.7 ± 2.2 $\mu g/m^3$ of PM_{10} are contributed by residual oil combustion, but this contribution might not be further resolved into concentrations attributable to Power Plant 2, Industrial Boiler 3, Hospital Heating Plant 6, etc. Sources which have similar chemical compositions cannot be separated by the model. The software performs tests on ambient data and source profiles which tell how well source-type contributions can be resolved from each other.

The CMB7 software can be applied to measurements of up to four different particle size fractions when source and ambient data are available. When

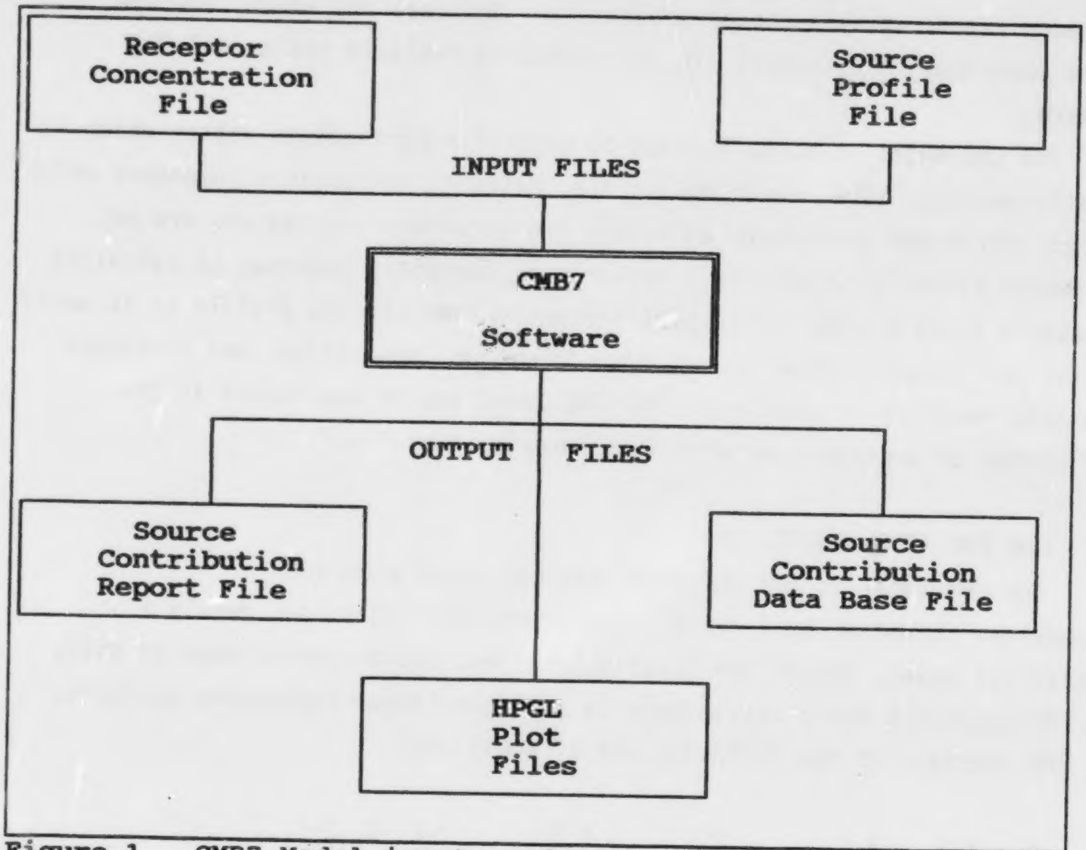
Receptor Concentration File
Source Profile File
INPUT FILES
CMB7 Software
OUTPUT FILES
Source Contribution Report File
Source Contribution Data Base File
HPGL Plot Files

Figure 1. CMB7 Model inputs and outputs.

modeling PM_{10}, the fine ($PM_{2.5}$, 0 to 2.5 μm aerodynamic diameter) and coarse (2.5 to 10 μm aerodynamic diameter) size fractions are often modeled separately. This feature allows particle size as well as chemical characteristics to be used in distinguishing one source type from another.

The CMB model calculates source contribution estimates for each individual ambient sample, which is usually of 24-hour duration for PM_{10}. The chemical profiles may differ from one sample to the next owing to differences in emission rates (e.g., some days may have wood-stove burning bans in effect and others will not), wind directions (e.g., a downwind point source would not be expected to be contributing at an upwind sampling site), and changes in emissions compositions (e.g., different gasoline characteristics and engine performance in winter and summer may result in different profiles). For PM_{10}

and every sample is apportioned separately. Seasonal and annual averages of source contribution estimates are calculated to evaluate the annual PM_{10} standard.

The CMB model is normally used to apportion particulate matter which is directly emitted. The remaining sulfate, nitrate, and organic compounds which are not attributed to primary emissions are secondary species and are not attributed directly to sources. Research is currently underway to calculate or measure fractionated source profiles which simulate the profile as it would look at the receptor after aging, transformation, deposition, and transport. When this research is completed, the CMB model may be applicable to the attribution of secondary as well as primary species.

1.2 HOW THE MODEL WORKS

The CMB model is derived from physical principles with assumptions stated in Appendix A. Therefore, the CMB is not purely a statistical model, though the least-squares estimation method used to solve the CMB equations bears resemblance to multiple linear regression analysis. The CMB consists of the following set of equations:

$$C_i = F_{i1}S_1 + F_{i2}S_2 + . . + F_{ij}S_j . . + F_{iJ}S_J \qquad i=1..I,\ j=1..J$$

where C_i = Concentration of species i measured at a receptor site

F_{ij} = Fraction of species i in emissions from source j

S_j = Estimate of the contribution of source j

I = Number of chemical species

J = Number of source types

These equations have a unique solution only when the number of species is equal to or greater than the number of sources. Model evaluation studies show that the greater the number of species, the more precise the apportionment. These simultaneous equations are solved by an effective variance weighted least squares estimation method (Watson et al., 1984) which has been thoroughly tested and documented. This method also requires variance weighted least squares estimation method (Watson et al., 1984) which has been thoroughly tested and documented. This method also requires precision estimates for the C_i and F_{ij} values as model input. These precision estimates result in realistic uncertainties associated with the source contribution estimates, S_j, which are calculated by the model. All source contribution estimates must be accompanied by their calculated standard errors when CMB modeling results are reported.

1.3 CMB SOFTWARE HISTORY

The Chemical Mass Balance (CMB) receptor model was first applied by Winchester and Nifong (1971), Hidy and Friedlander (1972), and Kneip et al. (1972). The original applications used unique chemical species associated with each source-type, the so-called "tracer" solution. Friedlander (1973) introduced the ordinary weighted least-squares solution to the CMB equations, and this had the advantages of relaxing the constraint of a unique species in each source-type and of providing estimates of uncertainties associated with the source contributions.

Gordon and his students at the University of Maryland (e.g., Kowalkzyk et. al., 1978) subsequently applied this method to many chemical species that they measured in source and receptor samples. The ordinary weighted least squares solution was limited in that only the uncertainties of the receptor concentrations were considered; the uncertainties of the source profiles, which are typically much higher than the uncertainties of the receptor concentrations, were neglected.

The first user-oriented software for the CMB model was programmed in 1978 at the Oregon Graduate Center in FORTRAN IV on a PRIME 300 minicomputer (Watson, 1979). The PRIME 300 was limited to 3 megabytes of storage and 64 kilobytes of random access memory. CMB Versions 1 through 6 updated this original version and were subject to many of the limitations dictated by the original computing system. CMB7 has been completely rewritten in a combination of the C and FORTRAN languages to operate on microcomputers with floating-point coprocessors, hard disk systems with tens of megabytes storage, and available memory of 640 kilobytes.

CMB 1 was used in the Portland Aerosol Characterization Study (PACS) to develop a State Implementation Plan for the control of Total Suspended Particulate Matter (Watson, 1979). This modeling was the first to identify and quantify residential wood combustion as a major contributor to particulate levels in a U.S. urban area.

Version 2 of the CMB software was installed on EPA's UNIVAC system in 1980. This model could be operated by direct dial-up from a remote terminal. The CMB 2 software was identical to CMB 1 except that the data input files were generalized. This version was used to introduce state and local pollution control agencies to receptor modeling in a series of workshops which were conducted during 1981.

CMB 3 included re-writing of the computer code in FORTRAN 77 and added a ridge regression solution to the effective variance least-squares estimation method for solving the CMB equations (Williamson and DuBose, 1983). This version operated on the EPA UNIVAC via remote terminals. The ridge regression algorithm was thought to reduce the effects of collinearity (i.e., two or more source profiles which are too similar to be separated from each other by the model) on source contribution estimates. Henry (1982) showed, however, that the ridge regression solution was equivalent to changing the source profiles from their measured values until the collinearity disappeared. He determined that the source contribution estimates given by the ridge regression solution did not represent reality, and its use for air quality modeling was abandoned.

CMB 4, created in 1984, ported the CMB 3 software to an IBM/XT microcomputer for the first time and added the original effective variance solution of CMB 1.

CMB Versions 2 through 4 were rarely used for air quality modeling owing to a lack of appropriate model input data, inadequate user instructions, and "buggy" software. The anticipation of a revised ambient air quality standard for suspended particulate matter, PM_{10}, resulted in a cooperative agreement between the U.S. Environmental Protection Agency and the Desert Research Institute of the University of Nevada System to re-package the software for regulatory applications.

CMB 5 was an experimental version which contained several solution methods, performance diagnostics, and output displays which could be easily evaluated by scientists and regulators via application to real and synthesized data sets. CMB 5 was revised nine times in response to recommendations and findings of these scientists and regulators. These individuals met in 1986 to finalize the software for regulatory applications and to prepare instructions for the use of this software in these applications. CMB 6.0 incorporated the recommendations of this group into software, a user's manual (U.S. EPA, 1987a), a protocol for applying and validating the CMB model (U.S. EPA, 1987b), and a protocol for reconciling CMB source apportionments with source apportionments determined by dispersion modeling (U.S. EPA, 1987c).

Even as CMB 6.0 was issued, its limitations were apparent. The computer code had never been intended for the capabilities of microcomputers. The data interfaces were inflexible and inconvenient, the memory allocation was inefficient, and the computational algorithms were slow. Advances in microcomputer memory, displays, and data analysis software created demands for more informative displays and easily transferrable model output formats. These limitations did not prevent the software from being applied in numerous PM_{10} source assessments which are described later in this update. Many recommendations were made by the users of CMB 6.0, and several software "bugs" (none of which were found to affect the source contribution estimates) were found. The user suggestions were compiled and have been addressed in CMB7.

1.4 DIFFERENCES BETWEEN CMB7 AND CMB 6.0

Many of the differences between CMB 6.0 and CMB7 software are internal. The algorithms and computer code have been rewritten in a combination of the C and FORTRAN languages to speed data access and calculations. The arrays have been expanded to accommodate a larger number of source types and receptor species. All of these changes are transparent to the normal user of the compiled computer code.

Several changes are external and affect the data input files, the output files, and the way in which the user interacts with the model:

- CMB7 is menu driven. The CMB 6.0 HELP command has been replaced by this menu. This feature removes the need to memorize command mnemonics and to enter them each time a model function is desired.

- Each set of source profile and receptor chemical concentrations may now be supplied to the model as a single, blank delimited ASCII record (data fields are distinguished by a blank between each field). These records are easily produced by popular data base and spreadsheet software. The option remains, however, to use CMB 6.0 source profile and ambient input file formats. (See discussions in Section 4.)

- Ambient concentration and source profile ID codes have been changed from two to six characters. This allows a much larger number of source profiles and chemical species to be used in the model. Input files for CMB 6.0 must be modified by inserting four blank spaces before the species or source-type code for each record in the input file. The date field has been expanded to eight characters from the six-character field length in CMB 6.0. (See Section 4 for details.)

- The optional INXXXXXX.IN7 input file which includes the names of other input data files can contain either five or seven filenames. To run CMB7 with CMB 6.0 input files, five input data filenames are listed in the same order as in CMB 6.0 with the *.DAT extension. To input data from constant record ASCII files (e.g., example files PRPORT.TXT and ADPORT.TXT), filenames in the sixth and seventh lines identify receptor and source profile files, respectively, and end with the *.TXT extender. The first five names may be blank or any filename without the *.DAT extension. (See Section 4 for details.)

- CMB7 uses dynamic memory allocation. CMB7 is no longer limited to 21 fitting species and 16 fitting sources as was CMB 6.0. All remaining memory up to 640K is available for use by the program. If fewer species are included, more profiles can be included. The precise number which can be used depends on the memory configuration of a given computing system. A number appears on the screen at the start of each session which indicates the size of the work array available to CMB7. A formula for the size of the work array required is given in Appendix A.

- CMB7 produces two output files: one similar to that of CMB 6.0 and another which contains the contribution of each source to each chemical species in a single, blank-delimited record. These records can be read directly into commonly used spreadsheet, data base, graphics, and statistical software.

- CMB7 produces pie charts of source contributions and bar charts of measured and calculated species concentrations. These graphics can be printed from the screen or directed to a file in HPGL language for high resolution printing or plotting.

- CMB7 produces the Modified Pseudo-inverse Matrix (MPIN) diagnostic to help identify the degree of influence each chemical species concentration has on the contribution of the corresponding source. (See Section 3 for details.)

1.5 ORGANIZATION OF USER'S MANUAL

Section 1 has stated the objectives of this User's Manual (this is a self-sufficient document) and identified the major differences between this version of CMB modeling software and its predecessor. The second section describes the software on the distributed EPA diskette, computer hardware requirements, and how to install CMB7 on IBM-compatible computing systems. The third section presents a tutorial using example files provided on the EPA disk. The fourth section describes the input and output files and methods of building input files. The final section describes the meaning and interpretation of different model outputs. The appendices describe the CMB model derivation from basic principles, the solution algorithms, model assumptions, and the results of tests of deviations from model assumptions.

SECTION 2
SOFTWARE INSTALLATION

This section describes the hardware requirements, computer programs, and installation procedures for CMB7.

2.1 HARDWARE AND OPERATING SYSTEM

The minimum requirements for running CMB7 software are:

- IBM PC compatible desktop, portable, or laptop computer
- Available random access memory in excess of 420K
- Single 5¼ dual-sided standard floppy disk drive
- DOS Version 2.0 or higher operating system

The recommended hardware configuration is:

- IBM compatible Intel 80286- or 80386-based microcomputer
- 640K random access memory
- Mathematical co-processor (Intel 8087, 80287, or 80387)
- EGA, VGA, or Hercules compatible video graphics adapter
- HP LaserJet II compatible laser printer
- DOS Version 3.0 or higher operating system
- Hard disk with a minimum of 20M bytes capacity

2.2 CMB SOFTWARE

CMB7 software can be acquired from the National Technical Information Service or it can be retrieved from the EPA's Support Center For Regulatory Air Models Bulletin Board System (SCRAM BBS). The software was developed under a cooperative agreement with the Desert Research Institute of the University of Nevada, an agency of the State of Nevada, and is non-proprietary. This software is written in the C and FORTRAN computer languages and is translated to an executable program using Microsoft (Microsoft Corp.,

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16011 NE 36th Way, Redmond, WA 98073) compilers. The source code is also available from the authors on written request accompanied by a formatted, double density 5¼" floppy disk. The standard disk contains the following files:

- CMB7.EXE: Executable code for CMB7.
- PROFIN.PRG: A dBaseIII+ or dBase IV utility program which selects data from EPA's Source Composition Library (U.S. EPA, 1988) for formatting into CMB7 input data files.
- CMBIN7.PRG: A dBase III+ or dBase IV utility program which converts dBase files into CMB7 input data file formats for source profile and ambient data.
- PROFILE.DBF: An example dBase source profile data file in EPA Source Composition Library format. The entire PROFILE.DBF file and its documentation (U.S. EPA, 1988) may be obtained from the U.S. EPA Office of Air Quality Planning and Standards.
- ADPORT.DBF: An example dBase ambient data file. This file may be used as an example format when requesting data from analytical laboratories.
- INPORT.IN7: An example input data file containing the filenames of all other example input files.
- POPORT.IN7: An example input data file containing species codes, mnemonics, and initial fitting species selections. POPORT.DAT is the CMB6 copy of this file which is used with the PROFIN program.
- SOPORT.IN7: An example input data file containing source profile codes, mnemonics, and initial fitting profile selections.
- ADPORT.TXT: An example input ambient data file in CMB7 format. This file can also be produced from the ADPORT.DBF file using the CMBIN7.PRG program.
- PRPORT.TXT: An example input source profile data file in CMB7 format. This file can also be produced from a PRPORT.DBF file (created with the PROFIN.PRG program) using the CMBIN.PRG program.
- ELNAM.STR and PROFILE.STR: These are dBase structure files which are used by the PROFIN.PRG program.
- MSHERC.COM: This utility program from Microsoft Corp. must be run prior to running CMB7 to obtain graphics output from a Hercules compatible video adapter.

- README.DOC: This file describes updates on software or the user's manual which are subsequent to the printing of this manual.

It is good practice to make a working copy of these programs on another floppy disk and to store the original disk in a safe location.

In addition to this non-proprietary software, several additional software packages have been found useful as a complement to CMB7:

- **EPA Source Composition Library (U.S. EPA, Office of Air Quality Planning and Standards, Air Quality Management Division, Non-Criteria Pollutant Programs Branch, MD-15, Research Triangle Park, NC 27711).** As noted above, this library and its documentation contain many source profiles compiled from several studies all over the U.S. The source profile data base is updated periodically, and new profiles may be submitted by CMB users to the data base at the stated address.

- **VEDIT PLUS (CompuView Products, Inc., 1955 Pauline Blvd., Ann Arbor, MI 48103).** This text editor is able to handle the long lines which can occur in CMB7 input files.

- **dBASE III+ or dBASE IV (Ashton-Tate, 20101 Hamilton Ave., Torrance, CA 90502).** This data base program is useful for assembling CMB7 input data files and for examining the OUXXXXXX.DT2 output files.

- **GRAFPLUS (Jewell Technologies, 4740 44th St. SW, Suite 203, Seattle, WA 98116).** This software product can be used to print screen graphic images on dot matrix printers.

- **PrintAPlot (Insight Development Corporation, 1024 Country Club Drive, Suite 140, Moraga, CA 94556).** This software product can be used to print the HPGL graphic files produced by CMB7 on dot matrix printers and HP LaserJet Series II laser printers.

- **Plotter in a Cartridge (Pacific Data Products, 6464 Nancy Ridge Drive, San Diego, CA 92121).** This hardware product can be used to print the HPGL graphic files produced by CMB7 on HP LaserJet Series II laser printers.

- **Harvard Presentation Graphics (Software Publishing Corporation, P.O. Box 7210, Mountain View, CA 94039).** Publication-quality pie charts, stacked bar charts, and time series plots can be produced from CMB7 output data using this plotting package.

The identification of commercially available software products does not constitute an advertisement or an endorsement of them. Data files can be constructed and the CMB model can be operated without proprietary software.

2.3 SOFTWARE INSTALLATION

It is assumed that the computing system has been properly configured using the instructions provided by its DOS systems manual. These instructions will vary from one computer to another. On a system without a hard disk, the systems disk must be inserted into the floppy disk drive to boot the system. After booting, the disk prompt (usually A> for a floppy disk system or C> for a hard disk system) appears on the display. All examples given here will assume that C> is the default prompt.

The default CONFIG.SYS file must be modified to provide sufficient buffer and file specifications. A 'FILES=14' and 'BUFFER=20' specification must appear in the CONFIG.SYS file. The values '14' and '20' are minimum values, and larger values are also acceptable. This modification may be made in a text editor or by using the following sequence of commands (computer prompts are in normal type, user responses are in **BOLD FACE**, and nonprinting responses are in parentheses):

```
C>  EDLIN CONFIG.SYS         (ENTER)
    I                        (ENTER)
    FILES = 14               (ENTER)
    BUFFERS = 20             (ENTER)
                             (CONTROL)(BREAK)
    E                        (ENTER)
```

The sequence above activates the DOS line editor (EDLIN), names the new file CONFIG.SYS, enters the Insert mode (I), increases the maximum number of files available to 14 and the number of buffers to 20, exits the Insert mode, and exits EDLIN. The system must then be rebooted using the following sequence:

```
C>                           (CONTROL)(ALT)(DEL)
```

On a hard disk system, the software is copied onto the disk using the following sequence of commands:

```
C>  MD CMB                   (ENTER)
C>  CD CMB                   (ENTER)
C>CMB>COPY A:*.*             (ENTER)
```

This sequence creates a directory entitled 'CMB', enters that directory, and copies all files from the program floppy disk in drive A to that directory. Before using the program, the command **C>CD CMB** should be entered to assure that operations are being performed in the proper directory.

With a single floppy disk drive, CMB7 may be executed with the program disk in Drive A from the A> prompt. After the program displays its first prompt, the program disk may be removed and another disk with the input files may be placed in drive A. Depending on the size of the input files, this disk may have limited space for CMB output files.

CMB input and output files may be read from and written to any disk drive by specifying the name of that drive in the filename. For example, specifying **B:ADPORT.TXT** will cause the software to seek this ambient data input file on drive B. This is especially useful when a system with two floppy disk drives is used.

The CMB7 software is now installed. The next section presents a tutorial using the CMB model with the example data files.

SECTION 3
CMB MODEL OPERATIONS

This section describes the CMB model commands and illustrates the use of these commands in a tutorial example. The tutorial uses the example input data files which are included with the executable code. This example was drawn from the Portland Aerosol Characterization Study (Watson, 1979), the first study in which receptor modeling was used for regulatory purposes. This example is identical to that used in the tutorial of EPA's Technical Series Volume III (U.S. EPA, 1987a).

3.1 CMB COMMANDS

CMB7 is menu driven, and all commands are invoked by typing the number corresponding to the desired action when the prompt is given. The following menu appears in CMB7 after each operation:

```
 1   Change Fitting Species
 2   Change Fitting Sources
 3   Select Samples
 4   Advance to Next Sample
 5   Calculate Source Contributions
 6   Perform Autofit
 7   Present Data
 8   Present Source Contributions
 9   Write CMB Information to Disk
10   Present Computed Averages of CMB Series
11   Present Source Profile or Receptor Concentrations
12   Write Source Contributions to Species to Disk
13   Graph
14   Present Normalized (over species) MPIN Matrix
15   Exit
```

The number of the desired action is entered after the prompt "Enter selection, Type the line number to select." These commands are described in the following sub-sections.

Preceding page blank

3.1.1 Change Fitting Species

Fitting species are those which are used in the calculation of source contribution estimates. Species which are not included in this calculation are termed floating species. The comparison of calculated and measured values for floating species is part of the model validation process (U.S. EPA, 1987b). Fitting species should be selected which are major or unique components of the source-types influencing the receptor concentrations.

The menu displays row number, species code, species name, and fitting flags for up to four particle-size ranges. Only the first column is used for a single particle-size range or non-particulate species. The software designates the first entry in the list as total mass and sets its fitting flag to 'T'. This first entry is never used as a fitting species. Species for which data are lacking have fitting flags set to 'M' and are not available as fitting species. Species are selected or deselected for the current size fraction by entering the appropriate row number in response to the prompt. A '*' designates a fitting species while a blank designates a floating species. The **ENTER** key is depressed without the entry of a row number to return to the command menu.

3.1.2 Change Fitting Sources

Fitting sources are those for which source contribution estimates are calculated. Several profiles may be available which represent the same source-type, but only one of these is usually used as a fitting source. Profiles of similar chemical composition are often found to be collinear when two or more are selected as fitting sources. Fitting sources are selected which represent the emissions most likely to influence receptor concentrations.

The menu displays row number, profile code, profile name, and fitting flags for up to four particle-size ranges. Only the first column is used for a single particle-size range or non-particulate species. Profiles are selected or deselected for the current size fraction by entering the appropriate row number in response to the prompt. A '*' designates a fitting profile and a blank designates a non-fitting profile. The **ENTER** key is depressed without the entry of a row number to return to the command menu.

3.1.3 Select Samples

A subset of samples may be selected for CMB source apportionment with this command. This is especially useful when only a single size range is desired, when the "Perform Autofit" command is used, or when the "Present Computed Averages" command is used.

The menu displays row number, sample ID, sampling date, sample duration, start hour, and size range. Samples are selected or deselected for the current size fraction by entering the appropriate row number in response to the prompt. A '*' designates a fitting sample, while a blank designates a sample which will be skipped. The ENTER key is depressed without the entry of a row number to return to the command menu.

3.1.4 Advance to Next Sample

This command places in current memory the data from the next sample on the "Select Samples" list. The current fitting sample is deselected when this command is used.

Note: It is important to use Commands 9 and 12 prior to this command to save the CMB results.

3.1.5 Calculate Source Contributions

An effective variance weighted least squares calculation is applied to the fitting species and profiles for the selected sample. Source contribution estimates, their standard errors, model performance measures, and measured and calculated species concentrations are displayed to allow an evaluation of the validity of the solution. Pace and Watson (U.S. EPA, 1987b) explain the use of the displayed performance measures and methods to validate a source apportionment calculation. This command may be invoked as many times as needed to test the effects of selecting different fitting species and profiles.

Note: Data are recorded on disk only when Commands 9 or 12 are invoked.

3.1.6 Perform Autofit

Autofit allows a single selection of fitting species and profiles to be applied to a selected list of samples without operator intervention. This feature is especially useful for model simulation testing and screening purposes. Autofit is equivalent to invoking Commands 5, 9, 12, and 4 in succession until the source contributions for all selected samples have been calculated.

3.1.7 Present Data

This command displays the same information calculated by Command 5 without recalculating the source contribution estimates. The data are displayed on three separate screens, and this command allows data in these screens to be reviewed without the delay caused by the least squares calculation. Command 5 should be invoked at least once before this screen is displayed for a given selection of fitting species, fitting profiles, and samples to assure that correct values are displayed.

3.1.8 Present Source Contributions

This command presents a screen display of the fractional contribution of each source-type to each chemical species. These results are useful when contributions to species other than total mass are desired. They also indicate which sources are the major and minor contributors to each chemical concentration.

3.1.9 Write CMB Information to Disk

This command writes the information displayed by Commands 5 or 7 to the disk file CMBOUT.DT1. This output can be sent to a printer using the DOS PRINT command to retain a permanent record of each CMB modeling session. In addition, a fit to size fraction "COARS" data (Command 5), followed by Command 9, followed by a fit to size fraction "FINE" data without an intervening change in fitting sources or species, followed again by Command 9, will result in data being written to CMBOUT.DT1 for size "TOTAL," formed by combining source contributions for the two size fractions. This is also true for fits to size fraction "FINE" followed by size fraction "COARS."

Command 9 can be used for every CMB trial to record the changes made throughout the session. It is usually used only to record the best and final fit of the sources to the ambient data. A hardcopy record of a working session can be made by simultaneously entering (CTRL)(Print Screen) at the beginning of the modeling session. The printer must be connected to the computer and on line. Pressing (CTRL)(Print Screen) a second time switches off continuous printing. A single screen of information can be printed by entering (SHIFT)(Print Screen).

Note: Not all computers are configured for screen dumps. Check your computer manual concerning this feature.

3.1.10 Present Computed Averages

This command is ordinarily invoked after Autofit (Command 6) to calculate averages and standard deviations of the source contributions from a series of samples. The screen display can be optionally directed to the OUXXXXXX.DT1 hardcopy file. This command can also be used after a series of interactive source apportionment calculations. All source contribution estimates written to disk will be included in the average.

3.1.11 Present Source Profile or Receptor Concentrations

This command produces a screen display of the source profiles and receptor concentrations. It is used to verify that the input data have been accurately read into the CMB7 software.

3.1.12 Write Source Contributions to Species to Disk

This command produces an output file, entitled OUXXXXXX.DT2, of source contributions which is convenient for computer manipulation. The output is not convenient for visual examination. The contribution of each source-type to each chemical species is written to a single data record for that species. Each field in the record is blank-delimited, and the file can be easily read into popular data base or spreadsheet software.

3.1.13 Graph

This command presents a menu for four graph types: 1) bar chart of calculated and measured receptor species concentrations; 2) bar chart of source profiles; 3) pie chart of source contributions to a single sample; and 4) pie chart of source contributions to PM_{10} (if fine and coarse size fractions have been apportioned). After selection the graph is displayed until the ENTER key is depressed. Graphs 1 and 2 display species identifiers along the x axis. When the species are too numerous to be displayed on a single screen, entering an 'R' will shift the display window to the right and entering an 'L' will shift the display window to the left. With an appropriate printer and computer interface, the screen image may be turned into hardcopy by depressing **(SHIFT)(Print Screen)** keys. After exiting the graphical display, the program asks whether a graphics file is desired. A 'Y' response results in a Hewlett-Packard Graphics Language (HPGL) file being written to disk. These files can be read directly into desktop publishing and graphics software.

3.1.14 Present Normalized (over species) MPIN Matrix

This command presents a screen display of the transpose of the normalized modified pseudo-inverse matrix (MPIN) as described by Kim and Henry (1989). The MPIN matrix consists of rows for each fitting species and columns for each fitting source. The entries in this matrix indicate the degree of influence each species concentration has on the contribution of the corresponding source and the standard error of that estimate. The normalized MPIN matrix values indicate the sensitivity of the source contribution and standard error estimates to individual species. When entries exceed 0.5, the source contribution is very sensitive to the corresponding species concentration. The MPIN values are used to determine model stability. If there is doubt about the accuracy or precision of influential species concentrations, then the standard errors calculated by the model may not represent the true uncertainty of the source contributions.

3.1.15 Exit

This command closes all files, terminates program execution and returns control to the DOS operating system. The program may also be terminated with a CTRL-C or CTRL-BREAK key sequence, but output data may be lost. The exit command should be used in all cases except those in which the program appears to be hung up.

3.2 EXAMPLE CMB APPLICATION

This subsection illustrates the use of CMB7 by using the example files which are supplied with the software. These instructions should be followed closely during practice sessions with the test data. A printout of the initial run with the test data set for PACS1 is presented in Appendix C. If any difficulties are encountered following the instructions in this subsection, Appendix C should be consulted. Several additional runs for the same site and sampling date should be performed to determine whether predictions can be improved by adding or deleting some fitting source(s) or species.

Instructions in this subsection are in large type while all computer inputs and outputs are in small type. User responses are in bold-face type.

First, enter the CMB sub-directory

```
C>CD CMB
```

Start the model by typing

```
C>CMB>CMB7
```

The first software response reminds you that all user input must be in upper case.

```
MAKE SURE THAT YOUR CAPS LOCK IS ON ! ! !
```

You are first asked for the name of the file which contains the names of the input data files. The contents and formats of these files are discussed in Section 4.

```
DISK FILE FOR INITIAL INPUT?
IF NOT ENTER CARRIAGE RETURN
IF SO ENTER NAME OF DISK FILE
INPORT.IN7
```

On this prompt, enter the name of the file to which you want your output data directed. The default name will be CMBOUT. It is good practice to name these files in such a way that they identify sampling site, season, and monitoring network. CMB7 supplies its own extensions to this filename, and any extensions added to this filename are ignored.

```
DO YOU WISH TO RENAME CMBOUT?
IF NOT ENTER A CARRIAGE RETURN.
IF SO ENTER THE FILE NAME.
OUPORT
```

The model name, date and software authors then appear. Check the EPA's Support Center For Regulatory Air Models Bulletin Board System (SCRAM BBS) if you have doubts about whether or not you are operating with the most recent version.

```
***************************************************************************
*                                                                         *
*              U. S. EPA CHEMICAL MASS BALANCE RECEPTOR MODEL             *
*                        *** IBM-PC CMB7 89338  ***                       *
*                                                                         *
*     EPA PROJECT MGRS: THOMPSON G. PACE III, PE                          *
*                       QUANG NGUYEN                                      *
*                       U.S. ENVIRONMENTAL PROTECTION AGENCY              *
*                       OFFICE OF AIR QUALITY PLANNING AND STANDARDS      *
*                       RESEARCH TRIANGLE PARK, NC                        *
*                       (919)-541-5585                                    *
*                                                                         *
*    PRINCIPAL AUTHOR:     DR. JOHN G. WATSON                             *
*                          DESERT RESEARCH INSTITUTE                      *
*                          UNIVERSITY OF NEVADA SYSTEM                    *
*                          (702)-677-3166                                 *
*    CONTRIBUTING AUTHORS:                                                *
*    DR. J.C. CHOW          MR. P.L. HANRAHAN       DR. N.F. ROBINSON     *
*    MR. J.E. CORE          DR. R.C. HENRY          DR. H.J. WILLIAMSON   *
*    MR. D.A. DUBOSE        MR. T.G. PACE           DR. L. WIJNBERG       *
*    MR. QUANG NGUYEN                                                     *
***************************************************************************
```

71168 (This number specifies the number of separate floating point values which can be accommodated by the remaining memory in your system. Appendix A provides a method of relating this value to the number of profiles and species which you can use in the program.)

The first prompt asks you to

```
Initialize size fraction by selecting receptor site
Strike enter to continue (ENTER)

  1 PACS1          08/13/77 24 0  COARS
  2 PACS1          08/13/77 24 0  FINE
  3 PACS2          01/24/78 24 0  COARS
  4 PACS2          01/24/78 24 0  FINE
  5 PACS3          08/07/77 24 0  COARS
  6 PACS3          08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 1
```

Enter the line number for each sample. In this case, select the sample identified on line 1 by typing 1, and the following display appears with an asterisk opposite line 1. The asterisk indicates that sample is selected for CMB modeling.

```
  1 PACS1          08/13/77 24 0  COARS *
  2 PACS1          08/13/77 24 0  FINE
  3 PACS2          01/24/78 24 0  COARS
  4 PACS2          01/24/78 24 0  FINE
  5 PACS3          08/07/77 24 0  COARS
  6 PACS3          08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 2
```

Select the fine particle sample which corresponds to the coarse particle sample.

```
  1 PACS1        08/13/77 24 0  COARS *
  2 PACS1        08/13/77 24 0  FINE  *
  3 PACS2        01/24/78 24 0  COARS
  4 PACS2        01/24/78 24 0  FINE
  5 PACS3        08/07/77 24 0  COARS
  6 PACS3        08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: (ENTER)
```

Press the ENTER key to return to the main menu.

```
  1 Change Fitting Species
  2 Change Fitting Sources
  3 Select Samples
  4 Advance to Next Sample
  5 Calculate Source Contributions
  6 Perform Autofit
  7 Present Data
  8 Present Source Contributions
  9 Write CMB Information to Disk
 10 Present Computed Averages of CMB Series
 11 Present Source Profile or Receptor Concentrations
 12 Write Source Contributions to Species to Disk
 13 Graph
 14 Present Normalized (over species) MPIN Matrix
 15 Exit

Type the line number to select: 5
```

Each of the commands described in Section 3.1 is executed by typing its corresponding line number. By typing '5', for example, the CMB calculation is made for the first selected sample. There is a short delay (which can sometimes be up to a minute if operating on an 8086 system without a math coprocessor or if there are many species and source types), and the source contribution display appears.

```
SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1       DATE: 08/13/77  CMB7 89338
SAMPLE DURATION        24      START HOUR       0       SIZE:    COARS
       R SQUARE       .97     PERCENT MASS    100.6
     CHI SQUARE      1.44               DF       13

  SOURCE
     * TYPE     SCE(UG/M3)     STD ERR       TSTAT
----------------------------------------------------
1       MARIN     10.6029       1.8240      5.8131
3       UDUST      9.5985       1.2616      7.6081
4       AUTPB      9.0906       1.3961      6.5112
5       RDOIL      9.7127       1.6108      6.0296
8       KRAFT     12.3265       7.9102      1.5583
11      ALPRO     11.0997       2.2441      4.9462
12      STEEL      8.1587       1.5239      5.3538
13      FERMN      9.8720       1.6165      6.1072
----------------------------------------------------
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
     80.0+-      8.0/      80.0+-     8.0/     160.0+-     11.3

Strike enter to continue
```

This display provides most of the information needed to determine the source contribution estimates, their standard errors, and the model performance measures. The interpretation of these measures for each display is discussed in Section 5 of this manual. To obtain the next display, press the **ENTER** key

(ENTER)

and the similarity/uncertainty cluster display appears. This display indicates those profiles which are similar to each other and might not be reliably resolved by the CMB model.

```
        UNCERTAINTY/SIMILARITY CLUSTERS  CMB7  89338       SUM OF CLUSTER SOURCES
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
Strike enter to continue
```

Press ENTER again

(ENTER)

and the species concentration display appears. This display compares the calculated to measured concentrations of each chemical species. The asterisks next to a species ID indicate that the species was used in the CMB calculation.

```
SPECIES CONCENTRATIONS -  SITE: PACS1        DATE: 08/13/77  CMB7  89338
SAMPLE DURATION        24      START HOUR       0         SIZE:    COARS
      R SQUARE        .97    PERCENT MASS    100.6
    CHI SQUARE       1.44              DF       13

SPECIES-------I---MEAS------------------CALC-------------RATIO C/M----RATIO R/U
C1      TOT   T  80.00000+-  8.00000  80.46161+-  6.36458  1.01+-  .13       .0
C9  -   F           .73400+-   .07300    .50073+-   .22362    .68+-  .31    -1.0
C11     NA    *   6.33000+-   .63300   6.07759+-   .47089    .96+-  .12     -.3
C12     MG    *   1.48000+-   .14800   1.48676+-   .52389  1.00+-  .37      .0
C13     AL    *   4.84000+-   .48400   4.40992+-   .55081    .91+-  .15     -.6
C14     SI    *   3.27000+-   .32700   3.38783+-   .15779  1.04+-  .11      .3
C16     S         2.50000+-   .25000   2.41256+-   .28216    .97+-  .15     -.2
C17     CL    *   4.67000+-   .46700   5.19693+-  1.07658  1.11+-  .26      .4
C19     K     *   1.12000+-   .11200   1.44197+-   .38620  1.29+-  .37      .8
C20     CA    *   1.52000+-   .15200   1.47195+-   .10333    .97+-  .12     -.3
C22     TI    *    .14000+-   .01400    .13692+-   .03204    .98+-  .25     -.1
C23     V     *    .27700+-   .02800    .34841+-   .07289  1.26+-  .29      .9
C24     CR    *    .00800+-   .00100    .24531+-   .11640  30.66+-15.05    2.0
C25     MN    *   2.47000+-   .24700   2.43813+-   .12229    .99+-  .11     -.1
C26     FE    *   5.41000+-   .54100   4.11644+-   .30571    .76+-  .09    -2.1
C28     NI    *    .77900+-   .07800    .63016+-   .11802    .81+-  .17    -1.1
C29     CU    *    .05000+-   .00500    .06613+-   .00683  1.32+-  .19     1.9
C30     ZN    *    .21400+-   .02100    .23739+-   .03413  1.11+-  .19      .6

Strike enter to continue  (ENTER)
```

Most of the CMB displays provide only a single screen of information at a time; the remaining information is obtained by depressing ENTER when this prompt is seen.

```
C35   BR   *   .52000+-   .05200   .51378+-   .15795    .99+-  .32    -.0
C82   PB   *  1.78000+-   .17800  1.93077+-   .27347   1.08+-  .19     .5
C201  OC   * 10.10000+-  1.01000  8.38185+-  1.29686    .83+-  .15   -1.0
C202  EC   *  1.68000+-   .16800  1.34287+-   .39741    .80+-  .25    -.8
C203  SO4  *  8.10000+-   .81300  8.11920+-  1.25659   1.00+-  .18     .0
C204  NO3  *  1.13000+-   .11300   .71048+-   .41362    .63+-  .37   -1.0
------------------------------------------------------------------------------
Strike enter to continue
(ENTER)
```

The main menu appears after each command has been fully executed. This menu will be abbreviated in the remainder of this tutorial to save space.

```
  1 Change Fitting Species
    . . .
    . . .
 15 Exit

Type the line number to select: 1
```

The CMB is an interactive model in which the user must judge which profiles or species are most appropriate for a given sample. Species may be eliminated if the measurements are suspect or if an unidentified source is suspected as being a major contributor to that species. The fitting species are changed by invoking Command 1.

```
              Sizes:  FINE  COARS
  1 C1      TOT       T     T
  2 C9      F
  3 C11     NA        *     *
  4 C12     MG        *     *
  5 C13     AL        *     *
  6 C14     SI        *     *
  7 C16     S
  8 C17     CL        *     *
  9 C19     K         *     *
 10 C20     CA        *     *
 11 C22     TI        *     *
 12 C23     V         *     *
 13 C24     CR        *     *
 14 C25     MN        *     *
 15 C26     FE        *     *
 16 C28     NI        *     *
 17 C29     CU        *     *
 18 C30     ZN        *     *
 19 C35     BR        *     *
 20 C82     PB        *     *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: U
```

An asterisk appears next to each species which is used for each fitting species. The selection shown here is a default which is defined in the POPORT.IN7 file. The fitting species and sources can be different for different size fractions. There is not enough room on the display for all of the available species, and entering 'U' shows the remaining portions of the species list.

```
               Sizes:  FINE  COARS
 5 C13      AL           *      *
 6 C14      SI           *      *
 7 C16      S
 8 C17      CL           *      *
 9 C19      K            *      *
10 C20      CA           *      *
11 C22      TI           *      *
12 C23      V            *      *
13 C24      CR           *      *
14 C25      MN           *      *
15 C26      FE           *      *
16 C28      NI           *      *
17 C29      CU           *      *
18 C30      ZN           *      *
19 C35      BR           *      *
20 C82      PB           *      *
21 C201     OC           *      *
22 C202     EC           *      *
23 C203     SO4          *      *
24 C204     NO3          *      *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 8
```

Entering an '8' causes the asterisk corresponding to coarse particle CL to be removed. Chlorine is no longer a fitting species for the coarse fraction data. The species must appear on the screen to be selected or deselected.

```
               Sizes:  FINE  COARS
 5 C13      AL           *      *
 6 C14      SI           *      *
 7 C16      S
 8 C17      CL           *
 9 C19      K            *      *
10 C20      CA           *      *
11 C22      TI           *      *
12 C23      V            *      *
13 C24      CR           *      *
14 C25      MN           *      *
15 C26      FE           *      *
16 C28      NI           *      *
17 C29      CU           *      *
18 C30      ZN           *      *
19 C35      BR           *      *
20 C82      PB           *      *
21 C201     OC           *      *
22 C202     EC           *      *
23 C203     SO4          *      *
24 C204     NO3          *      *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: (ENTER)

   1 Change Fitting Species
     . . .
     . . .
  15 Exit

Type the line number to select: 2
```

In the same way, Command 2 allows the fitting source profiles to be changed interactively.

```
         Sizes:  FINE  COARS
 1 1     MARIN    *     *
 2 2     CDUST
 3 3     UDUST    *     *
 4 4     AUTPB    *     *
 5 5     RDOIL    *     *
 6 6     VBRN1
 7 7     VBRN2
 8 8     KRAFT    *     *
 9 9     SULFT
10 10    HOGFU
11 11    ALPRO    *     *
12 12    STEEL    *     *
13 13    FERMN    *     *
14 14    CARBO
15 15    GLASS
16 16    CARBF
17 17    SO4
18 18    NO3
19 19    OC
20 20    EC

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 8
```

Entering an '8' causes the asterisk corresponding to the coarse KRAFT profile to be removed. KRAFT is no longer a fitting profile for the CMB calculation.

```
         Sizes:  FINE  COARS
 1 1     MARIN    *     *
 2 2     CDUST
 3 3     UDUST    *     *
 4 4     AUTPB    *     *
 5 5     RDOIL    *     *
 6 6     VBRN1
 7 7     VBRN2
 8 8     KRAFT    *
 9 9     SULFT
10 10    HOGFU
11 11    ALPRO    *     *
12 12    STEEL    *     *
13 13    FERMN    *     *
14 14    CARBO
15 15    GLASS
16 16    CARBF
17 17    SO4
18 18    NO3
19 19    OC
20 20    EC

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: (ENTER)
```

```
  1 Change Fitting Species
    . . .
    . . .
 15 Exit

Type the line number to select: 5
```

Command 5 is invoked to re-calculate the source contribution estimates after each change in fitting species, profiles, or samples.

```
NO CONVERGENCE AFTER  20 ITERATIONS.  ENTER A CARRIAGE RETURN TO VIEW RESULTS

(ENTER)
```

In this case, the combination of fitting species and sources yields a very unstable solution. Appendix A shows that the effective variance least squares estimation method is an iterative solution which converges on the most probable values. This convergence usually occurs in two to five iterations. If a solution hasn't converged after 20 iterations, then the selection of sources and species is not physically meaningful, and other selections must be made. This message is one of the many internal model validation tests which are built into CMB7 software. Notice that many of the other performance measures are outside of reasonable ranges cited in Section 5 in the displays below.

```
SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1       DATE: 08/13/77  CMB7  89338
SAMPLE DURATION          24      START HOUR       0          SIZE:    COARS
      R SQUARE          .90    PERCENT MASS     94.8
    CHI SQUARE         4.85              DF       12

  SOURCE
     * TYPE      SCE(UG/M3)     STD ERR       TSTAT
-----------------------------------------------------
1         MARIN      12.9724      2.0982      6.1826
3         UDUST      11.8115      1.2227      9.6603
4         AUTPB      11.1218      1.5084      7.3734
5         RDOIL      11.7584      2.0859      5.6371
11        ALPRO      13.6058      2.4641      5.5217
12        STEEL       -.3121       .2882     -1.0829
13        FERMN      14.8819      1.5638      9.5168
-----------------------------------------------------

MEASURED CONCENTRATION FINE/COARSE/TOTAL:
      80.0+-      8.0/      80.0+-      8.0/      160.0+-     11.3
Strike enter to continue  (ENTER)

       UNCERTAINTY/SIMILARITY CLUSTERS  CMB7  89338       SUM OF CLUSTER SOURCES
-------------------------------------------------------------------------------

-------------------------------------------------------------------------------
Strike enter to continue  (ENTER)

SPECIES CONCENTRATIONS -  SITE: PACS1         DATE: 08/13/77  CMB7  89338
SAMPLE DURATION          24      START HOUR       0          SIZE:    COARS
      R SQUARE          .90    PERCENT MASS     94.8
    CHI SQUARE         4.85              DF       12

SPECIES-------I---MEAS------------------CALC-------------RATIO C/M----RATIO R/U
C1      TOT    T  80.00000+-   8.00000  75.83980+-   3.68599    .95+-   .11     -.5
C9      F            .73400+-    .07300     .62178+-    .25880    .85+-   .36     -.4
C11     NA     *    6.33000+-    .63300    6.59115+-    .56393   1.04+-   .14      .3
C12     MG     *    1.48000+-    .14800    1.15164+-    .70809    .78+-   .48     -.5
C13     AL     *    4.84000+-    .48400    5.31604+-    .67496   1.10+-   .18      .6
C14     SI     *    3.27000+-    .32700    3.65624+-    .19443   1.12+-   .13     1.0
C16     S           2.50000+-    .25000    2.28332+-    .33567    .91+-   .16     -.5
C17     CL          4.67000+-    .46700    5.74261+-   1.30243   1.23+-   .30      .8
C19     K      *    1.12000+-    .11200    1.90394+-    .58130   1.70+-   .55     1.3
C20     CA     *    1.52000+-    .15200    1.14509+-    .11261    .75+-   .11    -2.0
C22     TI     *     .14000+-    .01400     .14879+-    .02506   1.06+-   .21      .3
```

```
C23   V     *    .27700+-    .02800    .41650+-    .08825  1.50+-  .35    1.5
C24   CR    *    .00800+-    .00100    .01272+-    .00580  1.59+-  .75     .8
C25   MN    *   2.47000+-    .24700   2.56464+-    .14741  1.04+-  .12     .3
C26   FE    *   5.41000+-    .54100   1.52394+-    .24114   .28+-  .05   -6.6
C28   NI         .77900+-    .07800    .65911+-    .14252   .85+-  .20    -.7
C29   CU    *    .05000+-    .00500    .04401+-    .00719   .88+-  .17    -.7
C30   ZN    *    .21400+-    .02100    .18275+-    .04540   .85+-  .23    -.6
C35   BR    *    .52000+-    .05200    .62465+-    .19393  1.20+-  .39     .5
C82   PB    *   1.78000+-    .17800   2.28533+-    .33450  1.28+-  .23    1.3
C201  OC    *  10.10000+-   1.01000   8.11789+-   1.36887   .80+-  .16   -1.2
C202  EC    *   1.68000+-    .16800   1.41114+-    .40161   .84+-  .25    -.6
C203  SO4   *   8.10000+-    .81300   7.95489+-   1.50170   .98+-  .21    -.1
C204  NO3   *   1.13000+-    .11300   1.02827+-    .50149   .91+-  .45    -.2
--------------------------------------------------------------------------------
Strike enter to continue (ENTER)

  1 Change Fitting Species
      . . .
      . . .
  15 Exit

Type the line number to select:
```

Re-select CL as a fitting species and KRAFT as a fitting profile by using Commands 1 and 2 as described above. The screen displays are not reproduced below.

```
  1 Change Fitting Species
      . . .
      . . .
  15 Exit

Type the line number to select: 9
```

To save results on disk in a hardcopy format which is identical to the three screen displays, enter Command 9 at the prompt. The screen display is written to the OUPORT.DT1 data file. Command 12 writes the contribution of each source profile to each chemical species concentration on a single, long record into the file OUPORT.DT2. It is a good idea to use both of these before proceeding to the next sample.

```
  1 Change Fitting Species
      . . .
      . . .
  15 Exit

Type the line number to select: 4
```

Since the coarse fraction apportionment is completed, it is time to perform the fine fraction apportionment. Command 4 brings the next sample's data into the model calculation arrays.

```
  1 Change Fitting Species
      . . .
      . . .
  15 Exit

Type the line number to select: 5
```

Command 5 once again calculates the source contribution estimates and presents the three displays of model results.

```
SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1       DATE: 08/13/77  CMB7  89338
SAMPLE DURATION        24       START HOUR        0          SIZE:     FINE
       R SQUARE       .98     PERCENT MASS      98.7
     CHI SQUARE      1.12               DF        13

  SOURCE
     * TYPE     SCE(UG/M3)     STD ERR       TSTAT
--------------------------------------------------
1       MARIN      12.3889      2.2457      5.5167
3       UDUST       9.5917      1.3876      6.9127
4       AUTPB      10.0835      1.4942      6.7486
5       RDOIL      11.0603      1.9239      5.7490
8       KRAFT       4.6896      5.0467       .9292
11      ALPRO      10.6023      3.5896      2.9536
12      STEEL       8.6729      1.3771      6.2979
13      FERMN      11.8754      1.8321      6.4820
--------------------------------------------------

MEASURED CONCENTRATION FINE/COARSE/TOTAL:
     80.0+-     8.0/     80.0+-     8.0/     160.0+-     11.3
Strike enter to continue  (ENTER)

       UNCERTAINTY/SIMILARITY CLUSTERS  CMB7  89338      SUM OF CLUSTER SOURCES
-------------------------------------------------------------------------------

       1     8                                           17.078+-      4.241
       1     5     8                                     28.139+-      3.833
-------------------------------------------------------------------------------
Strike enter to continue (ENTER)

SPECIES CONCENTRATIONS -  SITE: PACS1           DATE: 08/13/77  CMB7  89338
SAMPLE DURATION        24        START HOUR        0          SIZE:    FINE
       R SQUARE       .98     PERCENT MASS   .  98.7
     CHI SQUARE      1.12                DF       13

SPECIES-------I---MEAS------------------CALC-------------RATIO C/M----RATIO R/U
C1     TOT    T  80.00000+-   8.00000  78.96461+-   4.82449    .99+-  .12     -.1
C9     F            .88300+-    .08800    .67644+-    .24792    .77+-  .29     -.8
C11    NA     *   6.93000+-    .69300   6.97025+-    .56446   1.01+-  .13      .0
C12    MG     *    .43000+-    .04300   1.60951+-    .62627   3.74+- 1.50     1.9
C13    AL     *   4.66000+-    .46600   4.02418+-    .88919    .86+-  .21     -.6
C14    SI     *   3.02000+-    .30200   2.92212+-    .13329    .97+-  .11     -.3
C16    S          2.95000+-    .29500   3.02466+-    .31807   1.03+-  .15      .2
C17    CL     *   5.95000+-    .59500   5.69381+-   1.24836    .96+-  .23     -.2
C19    K      *   1.64000+-    .16400   1.73084+-    .46411   1.06+-  .30      .2
C20    CA     *   1.78000+-    .17800   1.43537+-    .11366    .81+-  .10    -1.6
C22    TI     *    .08300+-    .00800    .10088+-    .01630   1.22+-  .23     1.0
C23    V      *    .37200+-    .03700    .39757+-    .08308   1.07+-  .25      .3
C24    CR     *    .31500+-    .03200    .20976+-    .12151    .67+-  .39     -.8
C25    MN     *   2.99000+-    .29900   2.82844+-    .14115    .95+-  .11     -.5
C26    FE     *   4.53000+-    .45300   4.24446+-    .33269    .94+-  .12     -.5
C28    NI     *    .76500+-    .07700    .68246+-    .13428    .89+-  .20     -.5
C29    CU     *    .04400+-    .00400    .05274+-    .00510   1.20+-  .16     1.3
C30    ZN     *    .22500+-    .02300    .26786+-    .03966   1.19+-  .21      .9
C35    BR     *    .41900+-    .04200    .56133+-    .17386   1.34+-  .44      .8
C82    PB     *   2.53000+-    .25300   2.13749+-    .30300    .84+-  .15    -1.0
C201   OC     *   7.54000+-    .75400   8.50978+-   1.35632   1.13+-  .21      .6
C202   EC     *   1.42000+-    .14200   1.33579+-    .34012    .94+-  .26     -.2
C203   SO4    *  10.30000+-   1.03400   9.78819+-   1.47514    .95+-  .17     -.3
C204   NO3    *    .63800+-    .06400    .88402+-    .35938   1.39+-  .58      .7
-------------------------------------------------------------------------------
Strike enter to continue  (ENTER)
```

In this case, several potential collinearities have been identified by the similarity/uncertainty clusters. It may be necessary to group several of these source profiles into a common profile which represents several source sub-types. No further experimentation will be conducted in this tutorial. The CMB data are recorded to disk by using Commands 9 and 12 at the menu prompt.

```
 1 Change Fitting Species
    . . .
    . . .
15 Exit

Type the line number to select:  9   then 12
```

There are several commands which allow the user to learn more about his input data and the nature of the CMB least squares calculation. As an example, invoke Command 3 and select line 1, the PACS1 coarse particle fraction. Exit to the menu and use Command 5 to re-calculate the source contributions for these data. The display was presented previously and will not be repeated.

```
 1 Change Fitting Species
    . . .
    . . .
15 Exit

Type the line number to select:  11
```

Command 11 allows inspection of the data which have been read into the CMB program. This is useful for verifying that all input data files were correctly formatted and that the data were correctly retrieved by the software. It is also useful when a deficit or surplus of a certain species is found in the species concentrations display. The source profiles can be examined one by one, or as a group, in order to find profiles which contain significant quantities of these species.

```
WHAT DO YOU WANT TO SEE?
ENTER S FOR SOURCE PROFILE OR R FOR RECEPTOR CONCENTRATIONS.
S
DO YOU WANT TO LOOK AT THE WHOLE MATRIX?
IT IS 20 SOURCES BY 24 SPECIES
N
WHICH SOURCE DO YOU WANT?
GIVE SOURCE CODE
4
SOURCE: AUTPB
C1     TOT          1.0000  +-     .0000
C9     F             .0000  +-     .0001
C11    NA            .0000  +-     .0005
C12    MG            .0000  +-     .0050
C13    AL            .0110  +-     .0050
C14    SI            .0082  +-     .0030
C16    S             .0040  +-     .0013
C17    CL            .0300  +-     .0100
C19    K             .0007  +-     .0003
C20    CA            .0125  +-     .0050
C22    TI            .0000  +-     .0010
C23    V             .0000  +-     .0000
```

```
C24     CR              .0000  +-      .0001
C25     MN              .0000  +-      .0002
C26     FE              .0210  +-      .0080
C28     NI              .0002  +-      .0001
C29     CU              .0007  +-      .0003
C30     ZN              .0035  +-      .0013
C35     BR              .0500  +-      .0170
C82     PB              .2000  +-      .0300
C201    OC              .5000  +-      .1000
C202    EC              .0380  +-      .0140
C203    SO4             .0130  +-      .0040
C204    NO3             .0091  +-      .0030

Strike enter to continue
(ENTER)
WHICH SOURCE DO YOU WANT?
GIVE SOURCE CODE
(ENTER)
WHAT DO YOU WANT TO SEE?
ENTER S FOR SOURCE PROFILE OR R FOR RECEPTOR CONCENTRATIONS.
OR ARE YOU DONE?
D
```

At each of the prompts, enter 'S' for source profiles, 'R' for receptor data, 'Y' for yes, 'N' for no, or 'D' for done. The 'D' returns to the main menu.

```
   1 Change Fitting Species
     . . .
     . . .
  15 Exit

Type the line number to select: 8
```

Command 8 presents the fractional amount which each source contributes to each species. This information is also useful when trying to determine which profiles are responsible for major over- or under-predictions of the measured species.

```
                                 CALC SPECIES(PER SOURCE)
        INDIVIDUAL RATIO = --------------------------
                                MEAS SPECIES(ALL SOURCES)

                                   SOURCE CODE
  SPECIES    MARIN  UDUST  AUTPB  RDOIL  KRAFT  ALPRO  STEEL  FERMN
   TOT        .155   .120   .126   .138   .059   .133   .108   .148
   F          .000   .000   .000   .007   .000   .720   .000   .039
   NA         .715   .017   .000   .056   .086   .063   .016   .053
   MG        1.383   .290   .000   .000   .069   .690  1.311   .000
   AL         .000   .182   .024   .013   .003   .614   .012   .016
   SI         .000   .708   .027   .035   .002   .012   .144   .039
   S          .139   .012   .014   .499   .186   .050   .058   .068
   CL         .833   .000   .051   .000   .014   .024   .027   .008
   K          .106   .060   .004   .019   .043   .014   .049   .760
   CA         .097   .131   .071   .098   .000   .020   .302   .087
   TI         .000   .740   .000   .147   .003   .051   .209   .066
   V          .000   .006   .000  1.023   .000   .018   .014   .008
   CR         .000   .014   .000   .017   .042   .000   .578   .016
   MN         .000   .004   .000   .002   .000   .000   .252   .687
   FE         .000   .127   .047   .073   .012   .011   .613   .055
   NI         .000   .001   .002   .775   .008   .026   .079   .000
   CU         .000   .065   .167   .189   .022   .106   .552   .097
   ZN         .000   .047   .157   .197   .014   .007   .463   .306
   BR         .059   .005  1.203   .003   .015   .009   .000   .045
   PB         .000   .014   .797   .005   .000   .001   .026   .002
   OC         .000   .150   .669   .103   .011   .055   .000   .142
```

```
    EC          .000   .125   .270   .241   .007   .172   .000   .125
    SO4         .120   .004   .013   .517   .182   .045   .021   .048
    NO3         .000   .000   .144   .113   .000   .068   .000  1.061

Strike enter to continue  (ENTER)

   1 Change Fitting Species
     . . .
     . . .
  15 Exit

Type the line number to select: 14
```

Command 14 presents the transpose of the normalized MPIN matrix. This matrix shows the relative influence of each species on each source contribution. The species with the largest amount of influence is assigned a value of ±1, and species with values which exceed 0.5 are considered to be highly influential. If only one species is influential for a given source, it is extremely important that its ambient and source measurements are accurate and precise. The effects of influential species on the similarity/uncertainty clusters and source contribution estimates can be determined by adding or dropping this species as a fitting species.

```
                           TRANSPOSE OF SENSITIVITY MATRIX

                                       SOURCE CODE
SPECIES    MARIN   UDUST   AUTPB   RDOIL   KRAFT   ALPRO   STEEL   FERMN
NA           .99     .01    -.03    -.09     .14     .01    -.06     .01
MG           .21    -.05    -.04    -.04    -.07     .13     .18    -.08
AL          -.17    -.03    -.10    -.11    -.05    1.00    -.14     .01
SI          -.02    1.00    -.05    -.05     .04    -.14    -.19     .02
CL          1.00    -.02     .04     .12    -.36    -.04     .01    -.02
K           -.04     .05    -.03    -.05     .11    -.01    -.22     .46
CA           .28     .02     .03     .12    -.19    -.03     .39    -.06
TI           .00     .49    -.07     .08    -.03    -.02    -.07     .02
V            .23    -.04    -.06    1.00    -.40    -.04    -.19     .04
CR          -.10    -.07    -.03    -.12     .13    -.02     .33    -.12
MN          -.02    -.07    -.10    -.04    -.07    -.03    -.05    1.00
FE          -.08    -.12    -.05    -.14     .07    -.06    1.00    -.31
NI           .17    -.06    -.06     .87    -.32    -.02    -.09    -.00
CU          -.12    -.19     .09     .02     .05     .17     .67    -.18
ZN          -.02    -.09     .07     .09    -.02    -.05     .31     .10
BR           .01    -.02     .55    -.05     .03    -.04    -.07    -.01
PB           .00    -.04    1.00    -.06     .00    -.07    -.08    -.05
OC          -.04     .09     .61     .04     .01     .02    -.22     .11
EC          -.01     .03     .16     .17    -.07     .20    -.16     .09
SO4         -.66     .01    -.04     .04    1.00    -.04    -.16    -.01
NO3         -.00     .01     .03     .06    -.04     .04    -.19     .35

Strike enter to continue  (ENTER)

   1 Change Fitting Species
     . . .
     . . .
  15 Exit

Type the line number to select: 13
```

Command 13 provides a visual display of CMB information. Bar charts of calculated and measured chemical concentrations, bar charts of source profiles, and pie charts of source contribution estimates can be produced with this command. Upon typing command 13, a graphics menu appears.

```
  1                    Graph elemental concentrations
  2                           Graph source profiles
  3                      Graph source contributions
  4                                     Graph PM10
  5                                Exit graph menu

Type the line number to select or deselect 1
```

The plot shown in Figure 2 appears on the computer display. Note that this plot displays both the calculated and measured concentrations of each chemical species. Thick lines correspond to the measured concentrations, while thin lines and "*" indicate calculated and fitting elements, respectively. Typing **ENTER** returns the prompt

```
Hardcopy?  Y or N
Y
```

Entering 'Y' results in the plot written to a file in HPGL language. This is the language which drives Hewlett Packard Plotters and can be read by many graphics, word processing, and desktop publishing programs. Figure 2 was integrated into this manual from the CMBPLOT file using WordPerfect 5.0.

```
Plot file name cmbplot.001
```

After this prompt, the graphics menu reappears

```
  1                    Graph elemental concentrations
  2                           Graph source profiles
  3                      Graph source contributions
  4                                     Graph PM10
  5                                Exit graph menu

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu:   2
```

Entering selection 2 displays the source profiles available for plotting.

```
  1  1      MARIN
  2  2      CDUST
  3  3      UDUST
  4  4      AUTPB
  5  5      RDOIL
  6  6      VBRN1
  7  7      VBRN2
  8  8      KRAFT
  9  9      SULFT
 10  10     HOGFU
 11  11     ALPRO
 12  12     STEEL
 13  13     FERMN
 14  14     CARBO
 15  15     GLASS
 16  16     CARBF
 17  17     SO4
```

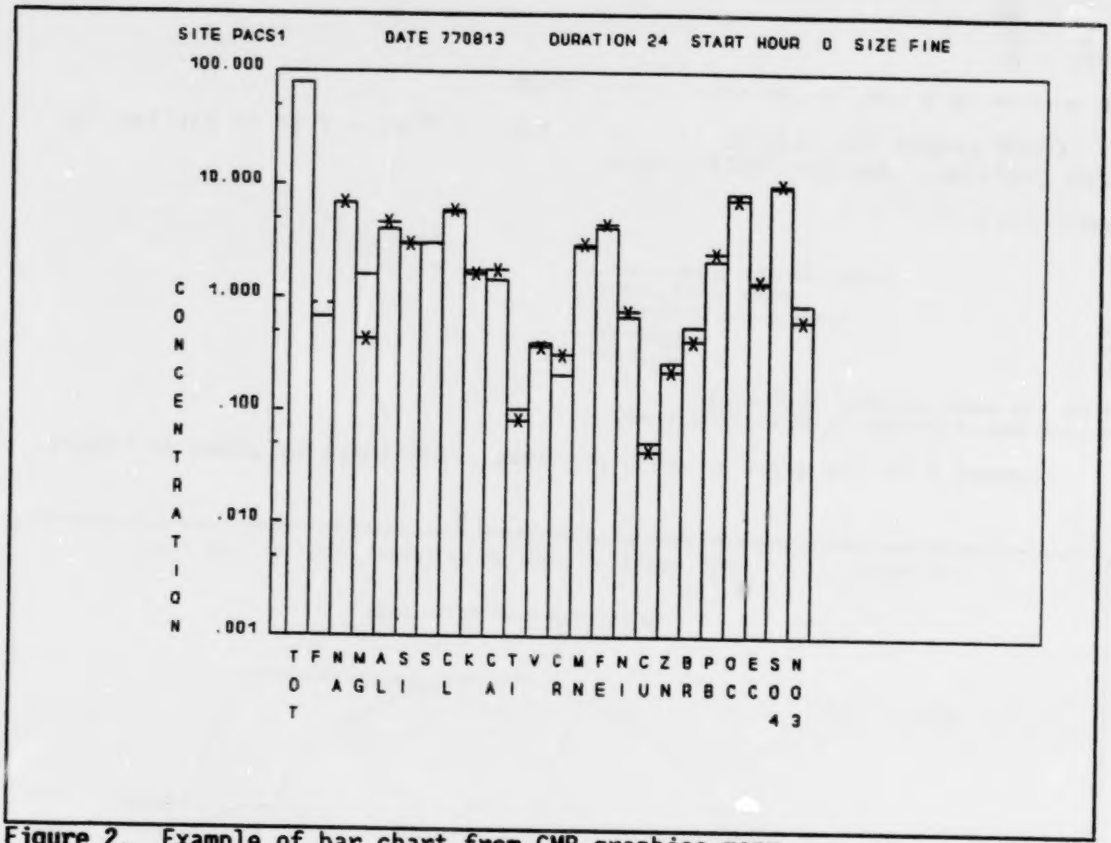

Figure 2. Example of bar chart from CMB graphics menu.

```
18  18      NO3
19  19      OC
20  20      EC

Toggle selection, Up or Down, Carriage return to exit:  4
```

Selecting source 4 causes an asterisk to appear beside this source profile mnemonic

```
 1   1      MARIN
 2   2      CDUST
 3   3      UDUST
 4   4      AUTPB      *
 5   5      RDOIL
 6   6      VBRN1
 7   7      VBRN2
 8   8      KRAFT
 9   9      SULFT
10  10      HOGFU
11  11      ALPRO
12  12      STEEL
13  13      FERMN
14  14      CARBO
15  15      GLASS
16  16      CARBF
```

```
   17  17      SO4
   18  18      NO3
   19  19      OC
   20  20      EC

Toggle selection, Up or Down, Carriage return to exit: (ENTER)
```

ENTER causes the display similar to that of Figure 2 to be plotted for source profiles. Another **ENTER** yields

```
Hardcopy?  Y or N
N

    1                    Graph elemental concentrations
    2                              Graph source profiles
    3                         Graph source contributions
    4                                         Graph PM10
    5                                    Exit graph menu

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 3
```

Command 3 in the graphics menu presents a pie chart as shown in Figure 3.

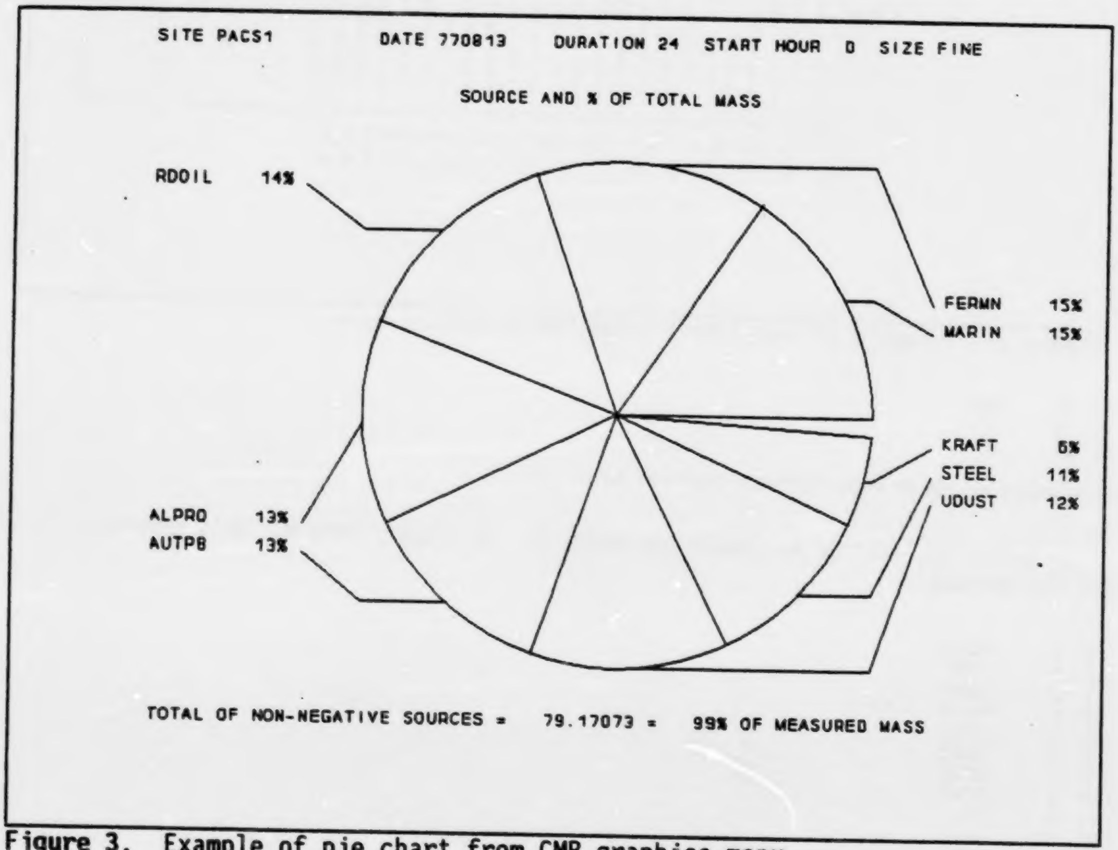

Figure 3. Example of pie chart from CMB graphics menu.

If both FINE and COARS particle-size ranges are included and have been apportioned, invoking Graphics Command 4 will plot a pie chart of the sum of these two fractions. Invoking Graphics Command 5 returns control to the main menu.

```
 1 Change Fitting Species
   . . .
   . . .
15 Exit

Type the line number to select:  6
```

It is often convenient to perform many CMB calculations at once and to record the data on disk without interaction. To accomplish this, we invoke Command 6, Autofit. Autofit allows a single selection of fitting species and profiles to be applied to a selected list of samples without operator intervention. This feature is especially useful for model simulation testing and screening purposes. Autofit is equivalent to invoking commands 5, 9, 12, and 4 in succession until the source contributions for all selected samples have been calculated. Autofit first preselects all samples and then enters Select Samples menu to allow deselection of any samples not to be included in the selected list.

```
 1 PACS1        08/13/77 24 0  COARS *
 2 PACS1        08/13/77 24 0  FINE  *
 3 PACS2        01/24/78 24 0  COARS *
 4 PACS2        01/24/78 24 0  FINE  *
 5 PACS3        08/07/77 24 0  COARS *
 6 PACS3        08/07/77 24 0  FINE  *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: (ENTER)
```

Exiting the Select Samples menu starts Autofit. There will be much disk activity but no screen displays until Autofit has completed its analysis. All of the CMB analyses may be printed from the OUPORT.DT1 and OUPORT.DT2 files.

```
 1 Change Fitting Species
   . . .
   . . .
15 Exit

Type the line number to select: 10
```

Command 10 creates a summary table of source apportionments for the series and calculates the average and standard deviation of the source contributions for each source profile used in the series.

```
OUTPUT WILL GO TO HARDCOPY.
DO YOU WANT IT DISPLAYED AT YOUR TERMINAL INSTEAD?
Y
```

The following output display can be directed to the OUPORT.DT1 file by entering 'N' instead of 'Y' at the prompt above.

```
CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------
PACS1         08/13/77  MARIN        12.39     10.60     22.99
PACS2         01/24/78  MARIN        -3.42       .31     -3.12
PACS3         08/07/77  MARIN        20.40     15.51     35.91
                                  --------  --------  --------
                         AVERAGE      9.79      8.81     18.60
                     (STD. DEV.)     12.12      7.76     19.88

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  UDUST         9.59      9.60     19.19
PACS2         01/24/78  UDUST         1.17     54.03     55.20
PACS3         08/07/77  UDUST        79.18     61.89    141.07
                                  --------  --------  --------
                         AVERAGE     29.98     41.84     71.82
                     (STD. DEV.)     42.82     28.20     62.62

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  AUTPB        10.08      9.09     19.17
PACS2         01/24/78  AUTPB        17.07      3.21     20.28
PACS3         08/07/77  AUTPB        23.93     35.26     59.19
                                  --------  --------  --------
                         AVERAGE     17.03     15.85     32.88
                     (STD. DEV.)      6.92     17.06     22.79

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  RDOIL        11.06      9.71     20.77
PACS2         01/24/78  RDOIL          .74       .19       .93
PACS3         08/07/77  RDOIL        14.01     12.45     26.46
                                  --------  --------  --------
                         AVERAGE      8.60      7.45     16.06
                     (STD. DEV.)      6.97      6.43     13.40

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  KRAFT         4.69     12.33     17.02
PACS2         01/24/78  KRAFT        14.23       .28     14.51
PACS3         08/07/77  KRAFT        -3.53      9.42      5.89
                                  --------  --------  --------
                         AVERAGE      5.13      7.34     12.47
                     (STD. DEV.)      8.89      6.29      5.84

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  ALPRO        10.60     11.10     21.70
PACS2         01/24/78  ALPRO         -.44      4.19      3.75
PACS3         08/07/77  ALPRO        -1.52      4.46      2.94
                                  --------  --------  --------
                         AVERAGE      2.88      6.58      9.46
                     (STD. DEV.)      6.71      3.91     10.61

CMB SITE       DATE      SOURCE       FINE     COARS     TOTAL
                                    (UG/M3)   (UG/M3)   (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         08/13/77  STEEL         8.67      8.16     16.83
```

```
PACS2         01/24/78   STEEL       -1.00       .56      -.45
PACS3         08/07/77   STEEL        -.02     -2.21     -2.23
                                   --------  --------  --------
                         AVERAGE      2.55      2.17      4.72
                      (STD. DEV.)     5.33      5.37     10.53

                                      FINE     COARS     TOTAL
CMB SITE      DATE       SOURCE     (UG/M3)   (UG/M3)   (UG/M3)
------------  --------   --------  --------  --------  --------

PACS1         08/13/77   FERMN       11.88      9.87     21.75
PACS2         01/24/78   FERMN         .62      -.11       .51
PACS3         08/07/77   FERMN         .09      1.41      1.50
                                   --------  --------  --------
                         AVERAGE      4.20      3.72      7.92
                      (STD. DEV.)     6.66      5.38     11.99

Strike enter to continue (ENTER)


  1 Change Fitting Species
    . . .
    . . .
  15 Exit

Type the line number to select: 15
```

All of the CMB menu commands have been illustrated in this tutorial, and the final Command 15 exits from the CMB modeling session.

```
C>
```

SECTION 4

INPUT AND OUTPUT DATA FILES

This section describes the structure of CMB7 input and output files and methods of generating these files.

4.1 CMB7 INPUT AND OUTPUT FILE DESCRIPTIONS

All CMB input and output files are named in the form PPXXXXXX.SSS.

- The PP prefix indicates the contents of the file.
- The XXXXXX is replaced by a user to identify the specific combination of data which he has placed in the file.
- The SSS extender indicates the format in which the data have been arranged.

For example, the filename INSNW7E1.IN7 could remind the user that this is the filename input file (IN) from the State of Nevada PM_{10} network (SN) fo winter (W) of 1987 (7) on EPA sampling days (E) at site 1 (1) in CMB7 text format (.IN7). The recommended prefixes and suffixes are identified in the descriptions of each individual file. A positioning line is situated above each example of input files to show where each field begins and ends. Some files are fixed format, which means that each field must begin and end on a certain column. Other fields are blank delimited, which means data fields are distinguished by one or more blank spaces between each field. Input data files described by U.S. EPA (1987a) in CMB 6.0 can be used in CMB7 with the following minor change:

- Insert four blank spaces before the element or source ID number in the POXXXXXX.DAT and SOXXXXXX.DAT.

This change can be made in a text editor (or a word processing program) and is needed because CMB7 views these numbers as six characters instead of

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two digits. Other than this change, the descriptions of CMB 6.0 input data files are fully described by U.S. EPA (1987a) and those descriptions will be briefly documented in Section 4.3. The CMB 6.0 formats should only be used if they already exist. All new CMB input files should be constructed according to the formats described in this document. CMB 6.0 formats will not be supported in subsequent versions of the CMB software.

4.1.1 Input Filename File: INXXXXXX.IN7

This fixed format file contains a list of the names of other CMB7 input data files. This filename, which is entered in response to the first prompt when the CMB software is started, consists of seven lines as shown below. Lines 1 through 3 contain any space filler such as 'XXXXXX'. Lines 4 through 7 contain the names of the files which are described in the following subsections. INPORT.IN7 is an example of this file structure used in CMB7.

```
File:  INPORT.IN7
0         1         2
12345678901234567890
Begin File:
XXXXXX
XXXXXX
XXXXXX
SOPORT.IN7
POPORT.IN7
ADPORT.TXT
PRPORT.TXT
End file.
```

Each filename can be up to eight characters in length with up to a three-character extender. Each filename in this input filename file must be left-justified and occupy Columns 1-12, Rows 4 through 7. The purpose of this file is to save the effort of keying in the input filename individually. If an INXXXXXX.IN7 filename is not entered at the prompt, CMB7 will request the names of individual data input filenames.

4.1.2 Source Profile Selection File: SOXXXXXX.IN7

The most commonly used source profiles are usually identified in initial CMB modeling sessions. It is often convenient to designate these profiles as defaults which will be selected each time the model is used. These default profiles can be designated in the SOXXXXXX.IN7 file. Each line of this file contains a six-character source code number in Columns 1 to 5 and an eight-character source profile name in Columns 9-16. Source codes need not be entered in numerical order, though this arrangement is helpful for file editing and documentation. If the source is to be included as an initial fitting source (as defined in Section 3.1.2), an asterisk is placed in Column 19. All other columns on each line are usually blank, but Columns 21-80 can be used for comments or source documentation which can be viewed during screen editing or when the file is printed. The maximum number of sources which can be used in CMB7 depends on several variables, as described in Appendix A. Fifty to 100 source profiles can be easily accommodated in most cases.

SOPORT.IN7 is an example of the source profile selection file.

```
File:  SOPORT.IN7
         1         2
12345678901234567890    Optional Comments
Example:

Begin File:
    1  MARIN     *      Marine Aerosol
    2  CDUST            Continental Dust
    3  UDUST     *      Urban Dust--Better than CDUST in urban cases.
    4  AUTPB     *      Leaded Auto Exhaust
    5  RDOIL     *      Residual Oil Combustion
    6  VBRN1            Vegetative Burning Profile 1
    7  VBRN2            Vegetative Burning Profile 2
    8  KRAFT     *      Kraft Paper Mill
    9  SULFT            Sulfite Paper Mill
   10  HOGFU            Hogged Fuel Boiler
   11  ALPRO     *      Aluminum Production
   12  STEEL     *      Steel Blast Furnace
   13  FERMN     *      Ferromanganese Furnace
   14  CARBO            Carborundum Furnace
   15  GLASS            Glass Furnace
   16  CARBF            Carborundum Furnace
   17  SO4              Single Constituent Sulfate
   18  NO3              Single Constituent Nitrate
   19  OC               Single Constituent Organic Carbon
   20  EC               Single Constituent Elemental Carbon
End File.
```

As noted in the example above, comments which describe the meaning of the source profile identifier can be entered in each record of this file after the 20th space to further describe the source mnemonic or the reason it was selected as a default value.

4.1.2 Species Selection File: POXXXXXX.IN7

The most commonly used fitting species are usually identified by initial CMB modeling. These can be selected in POXXXXXX.IN7 as defaults which will be selected as fitting species at model startup. This feature alleviates the need to select these species individually every time the model is used.

This file structure is similar to that of the Source Names file. A six-character species code is placed in Columns 1 to 6 and an eight-character species name is placed in Columns 9 to 16. An asterisk in Column 19 designates that species as a fitting species. When Column 19 is blank, the species is a floating species. The code '01' is reserved for particulate mass and CMB7 assigns the species name 'TOT' to this code. In order to maintain consistency with species coding in the EPA Source Profile Library, atomic numbers of elements are recommended to be used for elemental species. The total number of species which can be accommodated by CMB7 depends on several variables, as described in Appendix A. Fifty to 100 different species can be easily accommodated in most applications.

POPORT.IN7 is an example of the chemical species file.

```
File:  POPORT.IN7
         1         2
12345678901234567890   Optional Comments
Begin File:
    C1  TOT              Total Mass by Gravimetry
    C9  F                Water-soluble Fluoride by IC
   C11  NA        *      Sodium by Short-lived Neutron Activation
   C12  MG        *      Magnesium by INAA
   C13  AL        *      Aluminum by X-ray Fluorescence
   C14  SI        *      Silicon by XRF--Marker for dust
   C16  S                Sulfur by X-ray Fluorescence
   C17  CL        *      Chlorine by X-ray Fluorescence
   C19  K         *      Potassium by X-ray Fluorescence
   C20  CA        *      Calcium by X-ray Fluorescence
   C22  TI        *      Titanium by X-ray Fluorescence
   C23  V         *      Vanadium by X-ray Fluorescence
   C24  CR        *      Chromium by X-ray Fluorescence
```

```
    C25  MN      *      Manganese by X-ray Fluorescence
    C26  FE      *      Iron by X-ray Fluorescence
    C28  NI      *      Nickel by X-ray Fluorescence
    C29  CU      *      Copper by X-ray Fluorescence
    C30  ZN      *      Zinc by X-ray Fluorescence
    C35  BR      *      Bromine by X-ray Fluorescence
    C82  PB      *      Lead by X-ray Fluorescence
   C201  OC      *      Organic Carbon by TOR
   C202  EC      *      Elemental Carbon by TOR
   C203  SO4     *      Sulfate by Anion Chromatography
   C204  NO3     *      Nitrate by Anion Chromatography
End File.
```

Text comments can be added to this file after the 20th character to describe the species represented by the mnemonic. This is especially useful when the same species has been measured by different methods.

4.1.3 Ambient Data Input File: ADXXXXXX.TXT

The first record of the ADXXXXXX.TXT file contains identifiers for each field. These identifiers can be up to six alphanumeric characters in length and are separated by a blank. CMB7 software uses these identifiers in the order given in this file to identify species concentrations and their precisions in screen and output displays.

The ADXXXXXX.TXT file contains records with the following entries:

Field 1: Site ID (up to 12 characters)
Field 2: Sampling date (up to 8 characters)
Field 3: Sample duration (up to 2 characters)
Field 4: Sample start hour (up to 2 characters)
Field 5: Particle size fraction (up to 5 characters)
Field 6: Mass concentration (any number of characters in integer, floating point, or exponential format)
Field 7: Precision of mass concentration (same format as Field 6)
Field 8+2n: Concentrations of chemical species (same format as Field 6), where n = 0, 1, 2, ...
Field 9+2n: Precisions of species concentrations (same format as Field 6), where n = 0, 1, 2, ...

Data records containing the blank delimited fields (i.e., data fields are distinguished by a blank between each field) specified above follow this first record. The total number of records which can be included depends on the number of species, number of sources, and size of the computer memory. In most cases, one hundred or more records can be included in a single model input file.

Up to four different size fraction identifiers may be used, and the user can select mnemonics which suit his purposes. The size fraction names FINE and COARS are reserved for the PM$_{2.5}$ and coarse particle (PM$_{10}$-PM$_{2.5}$) size fractions which are most commonly measured in PM$_{10}$ source assessment studies. When these mnemonics are used, a separate output display is produced which sums the FINE and COARS source contribution estimates to provide the estimates for PM$_{10}$.

Missing values for chemical species are indicated by placing a -99. in the species concentration and precision fields. A species for which the value is missing cannot be used as a fitting species. Precisions which exceed zero must be assigned to all chemical concentrations which will be used as fitting species. CMB7 will return an error message when it finds zero or negative precisions.

ADXXXXXX.TXT files can be generated from dBASE III+ ambient data files by first modifying the structure to contain the fields identified above, then running the CMBIN7.PRG program (instructions in Section 4.2). Input files can also be generated from spreadsheet files by arranging columns in the specified order and using the spreadsheet's "print to disk" or "text output" options. These files can also be created in a text editor which allows the editing of very long records (VEDIT is such an editor). CMB7 file structures lend themselves to data which are already in data base or spreadsheet formats, however, and CMB 6.0 formats lend themselves more readily to data entry via text editor.

The ADPORT.TXT file is an example input ambient data file in CMB7 format.

4.1.4 Source Profile Data Input File: PRXXXXXX.TXT

The PRXXXXXX.TXT file contains records with the following entries:

Field 1: Profile number or source code (up to six characters)
Field 2: Source mnemonic (up to eight characters)
Field 3: Particle size fraction (up to five characters)
Field 4+2n: Fraction of species in primary mass of source emissions (floating point or exponential format), where n = 0, 1, 2, ...

Field 5+2n: Variability of fraction of species in primary mass of source emissions (same format as Field 4), where n = 0, 1, 2, ...

The first record of the PRXXXXXX.TXT file contains identifiers for each field. These identifiers can be up to six alphanumeric characters in length, are blank delimited, and must correspond to the identifiers used in the ADXXXXXX.TXT file. The order of the chemical species in the PRXXXXXX.TXT file must be the same as the order specified in the ADXXXXXX.TXT and POXXXXXX.IN7 files.

Data records containing the blank delimited fields specified above follow this first record. The total number of records which can be included depends on the number of species, number of sources, and size of the computer memory. In most cases, one hundred or more records can be included in a single model input file.

Up to four different size fraction identifiers may be used, and the user can select mnemonics which suit his purposes. These identifiers must correspond to those used in the ADXXXXXX.TXT file.

Missing values for chemical species in source files are replaced by a best estimate with a large variability. Default values of 0 for the fraction and .0001 for the variability are often chosen for species which are expected to be present in small concentrations. This indicates that the species is present in source emissions at a concentration less than .01%. A smaller value may be appropriate for certain source-types and species. A precision value which exceeds zero must be entered for all fitting species. CMB7 will return an error message when it detects precisions which are less than or equal to zero.

PRXXXXXX.TXT files can be generated from single record dBASE III+ source profile files by first modifying the structure to contain the fields identified above, then running the CMBIN7.PRG program (instructions in Section 4.2). Input files can also be generated from spreadsheet files by arranging columns in the specified order and using the spreadsheet's "print to disk" or "text output" options. These files can also be created in a text editor which allows the editing of very long records (VEDIT is such an editor). CMB7 file structures lend themselves to data which are already in data base or spreadsheet formats, however, and CMB 6.0 formats lend themselves more readily to data entry via text editor.

PRXXXXXX.DBF files can be generated from the EPA source composition library dBASE III+ file structures using the PROFIN.PRG program (instructions are in Section 4.2). The PRPORT.TXT file is an example of an input source profile data file in CMB7 format.

4.1.5 Hardcopy Output File: OUXXXXXX.DT1

The hardcopy output file presents the source contribution estimates, standard errors, model performance measures, and measured and calculated chemical species on a one-page display for each sample. The written display is identical to that which appears on the screen during an interactive modeling session. This output can be printed to hardcopy and bound in a modeling report. The file format is in ASCII text mode and is self-explanatory. Examples of output are given in Section 3.

4.1.6 Data Analysis Output File: OUXXXXXX.DT2

The data analysis output file records the contribution of each source-type to each chemical species in a single data record. Sample identifiers and model performance measures are also included in each record. All fields are blank-delimited. The file structure is:

Field 1: Species identifier
Field 2: Fitting flag; a '*' indicates that the species was a fitting species, while a '_' indicates that it was not
Field 3: Sampling site identifier
Field 4: Sampling date
Field 5: Sample start hour
Field 6: Sample duration
Field 7: Particle size fraction
Field 8: Measured species concentration
Field 9: Precision of measured species concentration
Field 10: R square value
Field 11: Chi square value
Field 12: Percent of measured mass
Field 13+2n: Source contribution estimate, n = 0, 1, 2, ...
Field 14+2n: Standard error of source contribution estimate, n = 0, 1, 2, ...

Fields 1 and 3 through 9 repeat model input data. Fields 2 and 10 through 12 provide information about the CMB calculation. The remaining fields correspond to each source profile in the PRXXXXXX.TXT file and contain the source contribution estimates and standard errors for these sources. A value of -99. is recorded when a profile was not used in the calculation.

The first record in this output file contains blank delimited field identifiers. All subsequent records contain data. Fields 13+2n and 14+2n are labeled with source codes and source contribution uncertainty columns are labeled with source names.

4.1.7 Graphics Output File: CMBPLOT.XXX

In addition to CMBOUT.DT1 and CMBOUT.DT2, CMB7 also gives the user the option to produce Hewlett-Packard Graphics Language (HPGL) plot files of the screen graphic displays. Each plot is placed into a separate file of the same name with the extension incremented by one (e.g., CMBPLOT.001, CMBPLOT.002, etc.).

These plots can be read directly into many graphics and desktop publishing packages. Publication-quality plots can also be produced from these files on HP 7470 and 7475 plotters, or HP LaserJet II printers, using software or hardware previously described in Section 2.1.

4.2 CREATING DATA INPUT FILES

There are three common methods of creating the CMB input files: manually entering the data in the correct format using a text editor or word processing program; editing existing input files with a text editor or word processing program; or transferring files from computerized data bases.

A text editor or word processor in text mode can be used to type entire input files. It is best to bring the example files into the editor, then insert the new values in the same locations as the existing values by using the editor in TYPEOVER mode. All spaces between fields should be entered with the space bar; tabs should not be set. Each line should be terminated with the ENTER key rather than using the wraparound feature present in many editors. No blank lines at the end of the file should be present. Completed files should be saved with an appropriate filename. EDLIN, the line editor supplied with MS/DOS or PC/DOS, may be used, but it is not convenient since it is not screen oriented.

If input data files have been prepared for other applications (e.g., source profiles may be common to several different data sets), then these files may be cut and pasted to produce the needed input data files. Because of differences in individual editing programs, the user is advised to consult the manual for the editing program to be used for directions on opening a copy of the existing file, deleting and adding material, saving the changes, and renaming the file.

Many source profile and ambient data sets are available in data base management formats. Selections of data, field names, and data structure can be easily made by the data base software.

4.2.1 Conversion of EPA Source Data Base Files

The dBASE III+ program PROFIN.PRG selects source profiles and species from the EPA source composition library data base and places these into a dBaseIII+ file which can then be formatted into an ASCII input file for CMB7. An example of the EPA source composition library is included in the PROFILE.DBF example data base. The following tutorial using this program requires the dBaseIII+ or dBase IV data management software.

The dBase software must reside in the same directory as the CMB files, or a path to the dBase software must be established with the DOS PATH command, to successfully implement file conversions.

First, start dBase and obtain the dot prompt

```
C>DBASE
.DO PROFIN
ENTER THE NAME OF THE ELEMENT NAME FILE: POPORT.DAT
ENTER THE NAME OF THE OUTPUT DBASE PROFILE FILE: PRPORT1
ENTER THE NAME OF THE EPA SOURCE PROFILE DBASE FILE: PROFILE
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 1
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 2
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 3
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 4
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 5
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 6
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 7
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 8
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 9
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 10
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 11
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 12
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 13
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 14
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 15
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 16
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 17
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 18
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 19
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: 20
ENTER THE PROFILE NUMBER OR A CARRIAGE RETURN TO EXIT: (ENTER)
. USE PRPORT1
. COPY TO PRPORT FOR SIZE='AO_25'.OR.SIZE='A2_10'
. USE PRPORT
. REPLACE SIZE WITH 'FINE' FOR SIZE='AO 25'
. REPLACE SIZE WITH 'COARS' FOR SIZE='A2_10'
. MODIFY STRUCTURE
```

Eliminate the fields 'Cl' and 'TOT' by placing the cursor on each one with the up arrow or down arrow key and pressing CTRL-U. Press CTRL-W to save these changes. Enter BROWSE and enter the desired source mnemonic in the name column. Save these changes by typing CTRL-W. The remaining dBase file should look like this:

```
CODE   NAME    SIZE        C9         F     ...    C204       NO3
1      MARIN   FINE   0.00000   0.00000     ...  0.00000   0.00000
                                            ...
20     EC      COARS  0.00000   0.00000     ...  0.00000   0.00000
```

The following commands will convert the dBase file (e.g., PRPORT.DBF), which was prepared by the PROFIN.PRG program, into a text file (e.g., PRPORT.TXT).

```
.DO CMBIN7
NAME OF DBASE INPUT FILE: PRPORT
NAME OF CMB INPUT FILE:  PRPORT
.
```

This PRPORT.TXT file is in CMB7 input data format. The ADPORT.TXT input data file may be created by the DO CMBIN7 command and typing ADPORT instead of PRPORT in response to the prompts.

4.3 CMB 6.0 FILES FORMATS

CMB 6.0 file formats are not as versatile or data-base oriented as CMB7 formats. They are still available for users who prefer them, however, and a brief documentation is provided here. The files are:

- INXXXXXX.DAT. List of other input data filenames
- SOXXXXXX.DAT. List of source profile numbers and names
- POXXXXXX.DAT. List of species numbers and names
- FSXXXXXX.DAT. Fine particle source profiles
- CSXXXXXX.DAT. Coarse particle source profiles
- DAXXXXXX.DAT. Fine and coarse particle ambient concentrations

Each file except the DAXXXXXX.DAT file contains a single line format (i.e., entries on sequential lines all have the same format). The formats for the six files are presented in separate subsections below. The notations A, I, and F refer to alphanumeric, integer, and floating-point formats, respectively. A floating-point format designated F8.6, for example, indicates that the field is eight characters wide and, if no decimal point appears in the field it is assumed that six characters are to the right of the implied decimal. Frequently, this decimal point is included in the data in a floating point field; in that case, the actual decimal location overrides the implied location in the "F" format. Data entries in the I format should always be right justified (i.e., aligned to the right side of the field).

The INXXXXXX.DAT file contains the names of the five other filenames in the following order:

```
File:  INPORT.DAT
0         1         2
12345678901234567890
Begin File:
FSPORT.DAT
CSPORT.DAT
DAPORT.DAT
SOPORT.DAT
POPORT.DAT
End File.
```

SOXXXXXX.DAT and POXXXXXX.DAT are identical to SOXXXXXX.IN7 and POXXXXXX.IN7 except that the species codes must be numeric, not alphanumeric.

The CSXXXXXX.DAT and FSXXXXXX.DAT files contain four required input fields plus an unstructured comment area to describe the data recorded in those fields. The format is:

<u>COLUMN</u>	<u>FORMAT</u>	<u>CONTENTS</u>
1-2	I2	Source code number
3-6	I4	Species code
9-16	F8.X	Fraction of fine (or coarse) source emissions from indicated species
19-26	F8.X	Uncertainty of fraction
27-80	A60	Can be used for comments; usually to identify size fraction, source name, and species

All source code numbers and species codes used in this file must be listed in the SOXXXXXX.DAT and POXXXXXX.DAT files.

The DAXXXXXX.DAT file contains two line formats for each sample. The header format (identified by the numbers 03 in columns 1 and 2) provides information on the receptor site and date and is limited to a single line. The second type of format (identified by the numbers 30 in columns 1 and 2) records ambient concentrations for the above site and date, with a separate line for each chemical species.

TYPE	COLUMN	FORMAT*	CONTENTS
Header	1-2	I2	'03'
	4-15	A12	Receptor identification
	17-18	A2	Year, YY
	19-22	A4	Month and day, MMDD
	24-25	I2	Duration of sample, hours
	27-28	I2	Starting hour of sample
	33-34	I2	Size fractions on next lines; 12 = fine and coarse; 13 = fine and total
	35-80		Must be blank
Concentration	1-2	I2	'30'
	4-15	A12	Receptor identification
	17-18	A2	Year, YY
	19-22	A4	Month and day, MMDD
	24-25	I2	Duration of sample, hours
	27-28	I2	Starting hour of sample
	31-34	I4	Species code
	37-45	F9.X	Concentration of fine fraction
	48-56	F9.X	Standard error of fine fraction (measurement uncertainty)
	59-67	F9.X	Concentration of coarse or total fraction
	70-78	F9.X	Standard error of coarse or total fraction (measurement uncertainty)

* I - Integer (I2; 0 through 99)
A - Alphanumeric (A12; up to 12 characters, A-Z, 0-9, any keyboard symbol)
F - Floating point (F9.X; up to 8 integers and a decimal point). Note: It is very helpful in reading the file to have the decimal points aligned vertically. A decimal point must be included in the field.

An unlimited number of ambient samples can be included in this file. Species codes must be the same in all files. Measurement precisions which exceed zero must be assigned to the ambient concentration data.

If only PM_{10} data are available, all fine particle concentrations should be set to zero and the "fine and total" designation (13) should be entered in columns 33-34 of the header record. CMB analyses should be performed only on the total size fraction.

SECTION 5

CMB PERFORMANCE MEASURES

This section describes the different performance measures which are used to evaluate the validity of source contribution estimates. Greater detail on the use of the performance measures is presented by U.S. EPA (1987b). The performance measures are presented in three separate displays when Commands 5 or 7 are invoked: 1) the source contribution display; 2) the uncertainty similarity cluster display; and 3) the species concentration display. Each of these displays is discussed below. The equations used to calculate these measures are presented in Appendix A.

5.1 SOURCE CONTRIBUTION ESTIMATES DISPLAY

An example of a source contribution table display is shown below:

```
SOURCE CONTRIBUTION ESTIMATES - SITE: PACS1      DATE: 08/13/77  CMB7  89338
SAMPLE DURATION        24     START HOUR      0        SIZE:    COARS
      R SQUARE        .97   PERCENT MASS  100.6
    CHI SQUARE       1.44             DF     13

 SOURCE
    * TYPE     SCE(UG/M3)    STD ERR      TSTAT
-----------------------------------------------
1      MARIN      10.6029     1.8240     5.8131
3      UDUST       9.5985     1.2616     7.6081
4      AUTPB       9.0906     1.3961     6.5112
5      RDOIL       9.7127     1.6108     6.0296
8      KRAFT      12.3265     7.9102     1.5583
11     ALPRO      11.0997     2.2441     4.9462
12     STEEL       8.1587     1.5239     5.3538
13     FERMN       9.8720     1.6165     6.1072
-----------------------------------------------
MEASURED CONCENTRATION FINE/COARSE/TOTAL:
    80.0+-    8.0/     80.0+-    8.0/    160.0+-    11.3
```

Source contribution estimates are the main output of the CMB model. The sum of these concentrations approximates the total mass concentration. Negative source contribution estimates are not physically meaningful, but they can occur when a source profile is collinear with another profile or when the source contribution is close to zero. Collinearity is usually identified in the similarity/uncertainty cluster display. When the absolute value of a positive or negative source contribution estimate is less than its standard error, the source contribution is undetectable. Two or three times the standard error may be taken as an upper limit of the source contribution in this case.

The standard errors reflect the precisions of the ambient data, the source profiles, and the amount of collinearity among different profiles. Standard errors should be reported with every source contribution estimate. The standard error is a single standard deviation. There is about a 66% probability that the true source contribution is within one standard error and about a 95% probability that the true contribution is within two standard errors of the source contribution estimate.

The T-statistic (TSTAT) is the ratio of the source contribution estimate to the standard error. A TSTAT value less than 2.0 indicates that the source contribution estimate is at or below a detection limit. Low TSTAT values for several source contributions may be caused by collinearities among their profiles; this will be indicated by the Similarity/Uncertainty Clusters.

The reduced chi square, degrees of freedom, R square, and percent mass are goodness of fit measures for the least squares calculation.

The chi square is the weighted sum of squares of the differences between the calculated and measured fitting species concentrations. The weighting is inversely proportional to the squares of the precisions in the source profiles and ambient data for each species. Ideally, there would be no difference between calculated and measured species concentrations and chi square would equal zero. A value less than 1 indicates a very good fit to the data, while values between 1 and 2 are acceptable. Chi square values greater than 4 indicate that one or more species concentrations are not well explained by the source contribution estimates. The degrees of freedom equal the number of fitting species minus the number of fitting sources. The degree of freedom is needed when statistical significance tests are applied to the reduced chi square value.

The R square is the fraction of the variance in the measured concentrations data which is explained by the variance in the calculated species concentrations. It is determined by a linear regression of measured versus model-calculated values for the fitting species. R square ranges from 0 to 1.0. The closer the value is to 1.0, the better the source contribution estimates explain the measured concentrations. When R square is less than 0.8, the source contribution estimates do not explain the observations very well with the given source profiles and/or species.

Percent mass is the percent ratio of the sum of the model-calculated source contribution estimates to the measured mass concentration. This ratio should equal 100%, though values ranging from 80 to 120% are acceptable. If the measured mass is very low (< 5 to 10 $\mu g/m^3$), this ratio may be outside of this range because the precision of the mass measurement is about 2 $\mu g/m^3$ (EPA sampling requirements are 5 $\mu g/m^3$ precision).

5.2 SIMILARITY/UNCERTAINTY CLUSTER DISPLAY

This display is shown below:

```
         UNCERTAINTY/SIMILARITY CLUSTERS  CMB7  89338     SUM OF CLUSTER SOURCES
--------------------------------------------------------------------------------

         1      8
         1      5      8                                 17.078+-     4.241
                                                         28.139+-     3.833
--------------------------------------------------------------------------------
```

The first column contains the clusters, one cluster on each row. Each cluster is identified by the code numbers associated with its source profile. The clusters are formed when: 1) two or more source profiles in an eigenvector derived from the singular value decomposition exceed 0.25 (these terms are explained in Appendix A); and 2) the T-statistic for any one of these source-types is less than or equal to 2.0. These uncertainty/similarity clusters are caused by excessive similarity (collinearity) among the source profiles in the cluster or by high uncertainties in the individual source profiles. The standard errors associated with the source contribution estimates of one or more sources identified in a cluster are usually very large, often too large to allow an adequate separation of these source contributions to be made.

If collinearity is the cause of these excessive standard errors, then the standard error of the sum of the source contributions for a cluster may be smaller than the standard error of any single source contribution in the cluster. The sum of source contributions and the standard error of the sum are shown in the final column of this display. This sum may be more useful than the individual source contribution estimates if the standard error of the sum is substantially lower than the standard errors of each source contribution estimate. The sum does not allow differentiation among the contribution estimates of the sources contained in the cluster.

Clusters will not appear if the two above-stated criteria are not met. This absence of clusters means that the source contributions can be resolved in the specific application. Since ambient data uncertainties, and relative levels of source contributions vary from sample to sample, it is possible that a given combination of profiles may appear in the clusters for one set of ambient data, but not for another set. For this reason, it is impossible to decide a priori that a set of profiles is collinear or not. The decision must be made for each set of data and each set of profiles combined with those data.

5.3 SPECIES CONCENTRATIONS DISPLAY

An example of the species concentration display is shown below:

```
SPECIES CONCENTRATIONS  -  SITE: PACS1          DATE: 08/13/77  CMB7  89338
SAMPLE DURATION        24       START HOUR       0          SIZE:    COARS
      R SQUARE        .90   PERCENT MASS      94.8
    CHI SQUARE       4.85             DF        12

SPECIES-------I---MEAS-------------------CALC--------------RATIO  C/M----RATIO R/U
C1      TOT   T  80.00000+-   8.00000  75.83980+-   3.68599    .95+-  .11   -.5
C9      F           .73400+-   .07300    .62178+-    .25880    .85+-  .36   -.4
C11     NA    *   6.33000+-    .63300   6.59115+-    .56393   1.04+-  .14    .3
C12     MG    *   1.48000+-    .14800   1.15164+-    .70809    .78+-  .48   -.5
C13     AL    *   4.84000+-    .48400   5.31604+-    .67496   1.10+-  .18    .6
C14     SI    *   3.27000+-    .32700   3.65624+-    .19443   1.12+-  .13   1.0
C16     S         2.50000+-    .25000   2.28332+-    .33567    .91+-  .16   -.5
C17     CL        4.67000+-    .46700   5.74261+-   1.30243   1.23+-  .30    .8
C19     K     *   1.12000+-    .11200   1.90394+-    .58130   1.70+-  .55   1.3
C20     CA    *   1.52000+-    .15200   1.14509+-    .11261    .75+-  .11  -2.0
C22     TI    *    .14000+-    .01400    .14879+-    .02506   1.06+-  .21    .3
C23     V     *    .27700+-    .02800    .41650+-    .08825   1.50+-  .35   1.5
C24     CR    *    .00800+-    .00100    .01272+-    .00580   1.59+-  .75    .8
C25     MN    *   2.47000+-    .24700   2.56464+-    .14741   1.04+-  .12    .3
C26     FE    *   5.41000+-    .54100   1.52394+-    .24114    .28+-  .05  -6.6
C28     NI         .77900+-    .07800    .65911+-    .14252    .85+-  .20   -.7
C29     CU    *    .05000+-    .00500    .04401+-    .00719    .88+-  .17   -.7
C30     ZN    *    .21400+-    .02100    .18275+-    .04540    .85+-  .23   -.6
C35     BR    *    .52000+-    .05200    .62465+-    .19393   1.20+-  .39    .5
C82     PB    *   1.78000+-    .17800   2.28533+-    .33450   1.28+-  .23   1.3
C201    OC    *  10.10000+-   1.01000   8.11789+-   1.36887    .80+-  .16  -1.2
C202    EC    *   1.68000+-    .16800   1.41114+-    .40161    .84+-  .25   -.6
C203    SO4   *   8.10000+-    .81300   7.95409+-   1.50170    .98+-  .21   -.1
C204    NO3   *   1.13000+-    .11300   1.02827+-    .50149    .91+-  .45   -.2
----------------------------------------------------------------------------------
```

This display shows how well the individual ambient concentrations are reproduced by the source contribution estimates. This display offers clues concerning which sources might be missing or which ones do not belong in the calculation. Fitting species are marked with an asterisk in the column labeled 'I'.

The column labeled RATIO R/U contains the ratio of the signed difference between the calculated and measured concentrations (the residual) divided by the uncertainty of that residual (square root of the sum of the squares of the uncertainty in the calculated and measured concentrations). The R/U ratio specifies the number of uncertainty intervals by which the calculated and measured concentrations differ. When the absolute value of the R/U ratio exceeds 2, the residual is significant. If it is positive, then one or more of the profiles is contributing too much to that species. If it is negative, then there is an insufficient contribution to that species and a source may be missing. The sum of the squared R/U for fitting species divided by the degrees of freedom yields the chi square. The highest R/U values for fitting species are the cause of high chi square values.

The column entitled RATIO C/M shows the ratio of calculated to measured concentration and the standard error of that ratio for every chemical species with measured data. The ratios should be near 1.00 if the model has accurately predicted the measured concentrations.

5.4 ADDITIONAL DIAGNOSTICS

Command 8 (Present Source Contributions) of the main menu produces a table that shows the fraction of each species' calculated ambient concentration contributed by each source in the fit. An example of this display is shown below:

```
                          CALC SPECIES(PER SOURCE)
     INDIVIDUAL RATIO = --------------------------
                          MEAS SPECIES(ALL SOURCES)

                                      SOURCE CODE
SPECIES   MARIN  UDUST  AUTPB  RDOIL  KRAFT  ALPRO  STEEL  FERMN
  TOT      .132   .121   .113   .102   .179   .138   .102   .124
  F        .000   .001   .000   .006   .000   .634   .000   .039
  NA       .667   .027   .000   .045   .120   .042   .016   .049
  MG       .343   .101   .000   .000   .000   .202   .359   .000
  AL       .000   .132   .021   .009   .008   .716   .011   .013
  SI       .000   .828   .023   .024   .006   .003   .125   .030
  S        .139   .000   .014   .436   .189   .000   .064   .067
  CL       .905   .000   .058   .000   .089   .028   .032   .009
  K        .132   .089   .006   .020   .051   .000   .067   .929
  CA       .097   .191   .074   .085   .034   .059   .333   .085
  TI       .000   .698   .000   .064   .000   .060   .117   .033
  V        .000   .009   .000  1.018   .000   .016   .018   .009
  CR       .000   .544   .000   .482  8.569   .221 21.456   .520
  MN       .000   .004   .000   .002   .003   .000   .288   .694
  FE       .000   .102   .035   .045   .049   .008   .483   .038
  NI       .000   .000   .002   .564   .040   .030   .073   .000
```

```
U        .000   .058   .132   .123   .171   .310   .458   .071
ZN       .000   .050   .148   .153   .000   .005   .458   .269
BR       .041   .001   .870   .002   .015   .026   .000   .031
PB       .000   .020  1.017   .005   .000   .000   .035   .003
OC       .000   .032   .448   .057   .223   .000   .000   .088
EC       .000   .089   .205   .151   .153   .105   .000   .089
SO4      .130   .001   .015   .487   .208   .023   .025   .051
NO3      .000   .002   .073   .047   .000   .000   .000   .500
```

The sources which are major contributors to each species can be determined by examining this display.

Another diagnostic is the transpose of the normalized modified pseudo-inverse matrix (MPIN). An example display of this diagnostic is shown below:

```
                     TRANSPOSE OF SENSITIVITY MATRIX

                                   SOURCE CODE
SPECIES    MARIN  UDUST  AUTPB  RDOIL  KRAFT  ALPRO  STEEL  FERMN
  NA       1.00    .01   -.04   -.06    .10   -.01   -.10    .03
  MG        .27   -.04    .02    .00   -.23    .10    .27   -.12
  AL       -.02    .02    .01    .00   -.18   1.00   -.22    .09
  SI       -.04   1.00   -.03   -.02    .03   -.12   -.20    .04
  CL        .78   -.03    .07   -.02   -.19   -.01    .05   -.05
  K         .01    .07   -.03   -.02    .09    .00   -.30    .52
  CA        .19    .05    .06    .08   -.20    .01    .54   -.15
  TI       -.01    .34   -.02    .03   -.03    .01   -.07    .02
  V         .10   -.04    .06   1.00   -.56    .02   -.06   -.01
  CR       -.17   -.06   -.12   -.15    .42   -.08    .29   -.14
  MN       -.03   -.06   -.05   -.04   -.10   -.00   -.03   1.00
  FE       -.04   -.12   -.05   -.06    .00   -.12   1.00   -.38
  U        -.26   -.12   -.06   -.09    .49    .25    .40   -.16
  ZN        .09   -.11    .14    .18   -.35   -.04    .50    .02
  BR        .09   -.02    .49    .02   -.19    .01   -.04    .01
  PB        .17   -.04   1.00    .06   -.45   -.00    .01   -.04
  OC       -.42    .07    .23   -.21   1.00   -.11   -.38    .14
  EC       -.19    .06    .03    .01    .40    .04   -.22    .09
  SO4      -.18    .01   -.16    .42    .62   -.07   -.29    .07
  NO3      -.01    .02    .03    .03   -.02    .01   -.16    .27
```

This matrix indicates the degree of influence each species concentration has on the contribution and standard of error of the corresponding source category. MPIN is normalized such that it takes on values from -1 to 1. Species with MPIN absolute values of 1 to 0.5 are associated with influential species. Noninfluential species have MPIN absolute values of 0.3 or less. Species with absolute values between 0.3 and 0.5 are ambiguous but should generally be considered noninfluential.

SECTION 6

SOURCE AND RECEPTOR PARTICULATE DATA BASES FOR THE CMB

One of the original objections to receptor modeling for PM_{10} source assessment was that source profile and ambient data were not available for their application. These objections are no longer valid, since a large number of data bases of both source and receptor measurements have been acquired in the United States for use in these models over the past decade. These data bases are widely dispersed, however, and are not generally available for study or evaluation. This situation is unfortunate because: 1) these existing particulate data bases might alleviate the need to acquire new data bases; 2) their potential for receptor model application and testing is untapped; 3) they provide models for success and failure which can enhance the design of new data acquisition projects; and 4) they provide a comprehensive view of particulate levels, concentrations, and source contributions for major parts of the United States. This section identifies several data bases which are available and can be used in the future to address these goals.

6.1 DATA BASE REQUIREMENTS

It is not possible, nor even of value, to catalog every measurement of particulate matter ever taken. Since many measurement programs have recently been completed, several are in progress, and others are planned, any compilation must be considered a snapshot at a particular time. Nevertheless, such a snapshot is useful since it provides a starting point for evaluating and using existing data. The information included here is useful today, and it will serve as a starting point for future compilations of a similar nature. The previous survey of this type was conducted for Total Suspended Particulate (TSP) data bases by Lioy et al. (1980) nearly a decade ago.

The ideal particulate matter data base for source and receptor measurements has the following characteristics:

- A large number of chemically and size classified concentrations. Mass, elements, ions, and carbon have been found to be the most easily measured and useful species, while PM_{10} and $PM_{2.5}$ are the most useful size ranges.

- Comprehensive coverage with respect to time, space, and, in the case of source samples, operating conditions. Simultaneous receptor samples taken at locations affected by different source-types are useful in the verification of receptor model source apportionments. Similarly, receptor samples taken in different seasons are affected by different emissions sources and meteorological conditions. Source samples need to represent the full range of profiles from a given source category so that uncertainties can be estimated for input to receptor models. Multivariate receptor models, such as multiple linear regression or factor analysis, require more than approximately 70 receptor samples to comply with their assumptions.

- Documentation of measurement methods, locations, and sampling times. Written records of the entire experimental program which acquired the data base are essential to its extended use. In the case of source characterization, this information should include the fuels, operating cycle, type of facility, location, and time of test.

- Quality control and quality audits. Replicates, field blanks, and independent verifications of field monitoring and laboratory operations are needed to assure that the stated procedures were actually complied with.

- Precision and accuracy estimates. State-of-the-art receptor modeling treats measurement uncertainties as part of the input data and returns uncertainties on source contribution estimates derived from those inputs. The quality control and quality audit data should be processed to quantify these uncertainties.

- Validation summaries or flags. Validation criteria should have been applied to every sample, and the results of that validation should be reported with the data.

- Availability in computerized formats. For research purposes, data cannot be proprietary or secret. If it is not in some computerized and documented form, preferably accessible by desktop computers, the expense of putting it into such form usually outweighs the potential benefits derived from examining the data.

6.2 DATA BASE SURVEY

The data bases presented here generally meet the foregoing requirements, though no single data base completely fulfills all of them. These data bases were identified via contacts with nearly 50 state and local agencies, universities, and researchers. Nearly 100 reports and publications were assembled and reviewed. The availability of the data in the public domain was ascertained, and data sets which could not be released were excluded from further consideration.

6.2.1 Source Characterization Data Bases

Table 1 summarizes the data bases which have been compiled for source profiles. The EPA source composition library (U.S. EPA, 1988) is recommended for Level I PM_{10} assessment. This library contains a large number of sources, but its current contents for motor vehicles and residential wood combustion are dated and do not reflect the compositions from modern vehicles, stoves, and fuels. The more recent source libraries (Cooper et al., 1987; Ahuja et al., 1989; Houck et al., 1989; Core et al., 1989; Watson et al., 1988, 1989) contain profiles which are more applicable to data bases acquired today for PM_{10} source assessment. The historical source libraries from the Portland Aerosol Characterization Study (Watson, 1979) and the wide range of profiles reported by Hopke (1985) are still of value because of their comprehensiveness and applicability to receptor data taken in an earlier era. Sheffield and Gordon (1986) present the most complete compilation of emissions characteristics from coal- and oil-fired power plants, and this is an excellent resource for studying pollution in areas with these source-types. Most of the collections of source profiles listed in Table 1 contain soil and road dust compositions, and it is unlikely that these profiles change over long periods of time. The Pacific Northwest Source Composition Library (Core, 1989) is one of the first to acquire speciation of the organic carbon fraction of source samples. The measurement of these additional species will allow them to be evaluated in receptor model applications to particulate matter.

6.2.2 Receptor Measurement Data Bases

Several major ambient particulate studies are described in Table 2. The notations are self-explanatory, and the reader is referred to the references for additional information on each study. All of those listed in Table 2 are

TABLE 1

SUMMARY OF CMB SOURCE PROFILES

Study (Reference)	Size Fractions	Major Source Types
EPA Receptor Model Source Library (Core et al., 1984; U.S. EPA, 1988)	0 - 2.5 μm 2.5 - 10 μm 0 - 10 μm 0 - 30 μm	Geological, Motor Vehicles, Vegetative Burning, Industrial
South Coast Air Basin Source Composition Library (Cooper et al., 1987)	0 - 2.5 μm 2.5 - 10 μm 0 - 10 μm	Geological, Motor Vehicles, Vegetative Burning, Industrial
California Air Resources Board Source Library (Ahuja et al., 1989; Houck et al., 1989)	0 - 1.0 μm 0 - 2.5 μm 0 - 10 μm 0 - 30 μm	Geological, Diesel Trucks, Vegetative Burning, Industrial
Pacific Northwest Composition Library (Core et al., 1989)	0 - 2.5 μm 2.5 - 10 μm	Geological, Motor Vehicles, Vegetative Burning, Industrial (Forest Products)
Receptor Modeling in Environmental Chemistry (Hopke, 1985)	0 - 2.5 μm 0 - 10 μm 0 - 30 μm	Geological, Motor Vehicles, Vegetative Burning, Industrial
Fine Particle Emissions from Stationary and Miscellaneous Sources in the South Coast Air Basin (Taback et al., 1979)	0 - 2.5 μm	Industrial
University of Maryland Source Compositions (Sheffield and Gordon, 1986)	0 - 2.5 μm 2.5 - 15 μm 0 - 30 μm	Coal- and Oil-Fired Power Plants
Portland Aerosol Characterization Study (Watson, 1979)	0 - 2.5 μm 0 - 30 μm	Geological, Wood Burning, Industrial
Montana Source Composition Library (Houck et al., 1982; 1984; Pritchett et al., 1985)	0 - 2.5 μm 2.5 - 15 μm 0 - 30 μm	Geological, Motor Vehicles, Wood Burning, Industrial

TABLE 1 (continued)

SUMMARY OF CMB SOURCE PROFILES

Study (Reference)	Size Fractions	Major Source Types
Missoula City-County Air Pollution Control District Source Library (Houck et al., 1987)	0 - 2.5 μm 2.5 - 10 μm	Geological, Motor Vehicles, Wood Burning
Wyoming Source Composition Library (Pritchett and Cooper, 1985a)	0 - 2.5 μm 2.5 - 15 μm	Geological
Alaska Source Composition Library (Pritchett and Cooper, 1985b)	0 - 2.5 μm 2.5 - 10 μm	Geological, Wood Burning
Harvard Air Pollution Health Effects Study (Chow, 1985)	0 - 2.5 μm	Geological
State of Nevada Air Pollution Study (Watson et al., 1988a)	0 - 2.5 μm 0 - 10 μm	Geological, Motor Vehicles, Wood Burning
SCENIC Denver (Watson et al., 1988b)	0 - 2.5 μm 0 - 10 μm	Geological, Motor Vehicles, Wood Burning, Industrial (brewery, catalyst cracker), Power Plant (coal and gas)

fairly major studies which were initiated for the purpose of applying receptor models, and several of the references include the results of the modeling. Hopke (1985) identifies a number of additional studies which are more short-term than the applications orientation of the data bases cited in Table 2.

TABLE 2

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
1. "STACS" - Seattle Tacoma Aerosol Characterization Study (Cooper et al., 1985)	• Urban sites in Washington • 10/82 to 12/82, 2/83 to 3/83, 1/84 to 3/84	• 24-hour samples for 0-2.5, 2.5-10 and 0-30 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance was applied for SIP development.
2. State of Washington Dept. of Ecology Monitoring Program (Beck and Associates, 1984)	• 3 sites in Washington • 5/83 to 10/83	• 24-hour samples for 0-2.5 and 2.5-10 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance and factor analysis were applied.
3. "PANORAMAS" - Pacific Northwest Regional Aerosol Mass Apportionment Study (Core et al., 1987)	• 7 sites in Washington, 5 sites in Oregon, 4 sites in Idaho • 5/84 to 9/84	• 24-hour and 12-hour samples for 0-1.5 and 0-2.2 μm size ranges and analyzed for mass, elements, ions, and carbon. • Concurrent visibility measurements are also available for source apportionment. Chemical mass balance was applied.
4. "PACS" - Portland Aerosol Characterization Study (Watson, 1979)	• 6 sites in Oregon • 4/77 to 4/78	• 24-hour, 8-hour, and 4-hour samples for 0-2.5 and 0-30 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance was applied for SIP development.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
5. "MACS" - Medford Aerosol Characterization Study (DeCesar and Cooper, 1980)	• 6 sites in Oregon • 4/79 to 3/80	• 24-hour samples for 0-2, 0-2.5, and 0-30 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance was applied.
6. "ACHEX" - Aerosol Characterization Experiment (Hidy et al., 1975)	• 11 sites in California • 7/72 to 11/72 7/73 to 10/73	• Six 2-hour samples were collected daily and analyzed for mass, elements, ions, and carbon. Concurrent meteorological measurements are also available. • Chemical mass balance was applied.
7. "SCAQS" - Southern California Air Quality Study (Blumenthal et al., 1987)	• 9 major sites in Los Angeles Area • 11/86, 6/87, 7/87 to 8/87, 11/87 to 12/87	• 24-hour and 4-hour samples for 0-2.5, 0-10, and 0-30 μm size ranges and analyzed for mass, elements, ions, carbon, carbonyls, hydrocarbon, etc.
8. "RESOLVE" - Research on Operations - Limiting Visual Extinction (Trijonis et al., 1987)	• 8 sites in SE Desert of California • 8/83 to 8/85	• 24-hour samples for 0-2.5 and 0-10 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance and other receptor modeling techniques were applied to attribute the visibility degradation in the Mohave Desert.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
9. California Particulate Study (Flocchini et al., 1976)	• 14 sites in California • 6/73 to 7/75	• 24-hour samples for 0.1-0.65, 0.65-3.6, and 3.6-20 μm size ranges and analyzed for mass and elements.
10. "WOGA" - Western Oil and Gas Association Aerosol Data Base (Watson et al., 1987b)	• 27 sites in California • 1/79 to 12/82	• 24-hour samples for 0-2.5, 2.5-15, 2.5-10, 0-3.5, and 3.5-40 μm size ranges and analyzed for mass, elements, and ions. This data base includes data collected from U.S. EPA and California Air Resources Board.
11. California Air Resources Board Dichotomous Sampling Network (Watson et al., 1987a)	• 7 sites in California • 1/80 to 12/82 1/83 to 6/86	• 24-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass and elements. • Chemical mass balance and factor analysis were applied.
12. South Coast Air Quality Management District PM$_{10}$ Studies (Gray et al., 1988)	• 7 sites in Southern California • 8/85 to 7/86 8/86 to 12/86	• 24-hour samples for 0-2.0 and 0-10 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance was be applied for SIP development.
•	• 3 sites in Riverside, California • 1/88 to 12/88	• 24-hour samples will be collected for 0-2.5 and 0-10 μm around Riverside, CA, and will be analyzed for mass, elements, ions, and carbon.

Table 2 (continued)

Ambient Particulate Data Bases

Study and Reference	Site Location and Study Period	Study Description
13. "SNAPS" - State of Nevada Air Pollution Study (Chow et al., 1988)	• 5 sites in Nevada • 1/86 to 3/87	• 24-hour and 6-hour samples for 0-2.5 and 0-10 μm size ranges and analyzed for mass, elements, ions, and carbon. • Chemical mass balance was applied.
14. Southern California Edison Cottonwood Cove Study (Bowen et al., 1986)	• Cottonwood Cove, NV • 1/81 to current	• 24-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass and elements.
15. East Helena Source Apportionment Study (Houck et al., 1984)	• 11 sites in Montana • 1/81 to 4/82	• 24-hour samples for 0-2.5, 2.5-15, and 0-30 μm size ranges and analyzed for mass, elements, and carbon. • Chemical mass balance was applied.
16. Kalispell, Montana Source Apportionment Study (Olsen, 1987)	• Kalispell, Montana • 6/86 to 5/87	• 24-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass, elements, and carbon. • Chemical mass balance was applied.
17. Arizona Statewide PM_{10} SIP Development (DeNee and Neuroth, 1988)	• 7 sites in Arizona • 9/87 to 9/90	• 24-hour and sporadic 4-hour samples for 0-2.5 and 2.5-10 μm size ranges and analyzed for mass, elements, and carbon. • Chemical mass balance was applied for SIP development.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
18. "VISTTA" - Visibility Impairment due to Sulfur Transport and Transformation in the Atmosphere (Blumenthal et al., 1981; Cahill et al., 1981 ; Hering et al., 1981; Macias et al., 1981a; 1981b)	• 2 sites in Arizona, 2 sites in Illinois • 6/79 to 7/29, 12/79, 2/81, 8/81 to 9/81	• 24-hour samples for 0-2.5 and 2.5-15 size ranges and analyzed for mass, elements, ions, and carbon. Concurrent meteorological measurements are also available.
19. 1978 Denver Winter Haze Study (Heisler et al., 1980)	• 6 sites in Colorado • 11/78 to 12/78	• 4-hour samples for 0-2.5, 2.5-15, and 0-30 μm size ranges and analyzed for mass, elements, ions, and carbon. Concurrent visibility measurement is also available. • Chemical mass balance and other receptor modeling techniques were applied.
20. "SCENIC" Denver" - Study Cooperative for Emissions and Impact Characterization in Denver (Watson et al., 1988B)	• 6 sites in Colorado • 11/87 to 2/88	• 7 and 17-hour day/night samples for 0-2.5 μm size range and analyzed for mass, elements, ions, and carbon. Concurrent meteorology and visibility measurements are also available. • Chemical mass balance and other receptor modeling techniques will be applied to assess the effect of visibility degradation due to emission changes.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
21. "AWVS" - The Albuquerque Winter Visibility Study (Zak et al., 1984)	• 3 sites in New Mexico • 12/82 to 2/83	• 12-hour daily samples for 0-2.5 and 2.5-10 µm size ranges and analyzed for mass, elements, ions, and carbon. • Multiple linear regression techniques were applied.
22. North Dakota Study (Schock et al., 1979)	• 4 sites in North Dakota • 5/87 to 10/87	• 24-hour daily samples were collected with stacked filter units (0-2.0 µm) and analyzed for mass and elements.
23. "RAPS" - Regional Air Pollution Study (Loo et al., 1978; Dzubay, 1980)	• 10 sites in Missouri • 5/75 to 3/79	• 6-hour and 12-hour samples for 0-2.5 and 2.5-15 µm size ranges and analyzed for mass and elements. • Chemical mass balance and other receptor modeling techniques were applied.
24. "SCENES" - Study Cooperative Electric Utility, Department of Defense, National Park Service, and Environmental Protection Agency Study (Mueller et al., 1986; McDade et al., 1989)	Regional Scale: • 9 sites in California, 3 sites in Nevada, 3 sites in Utah, and 4 sites in Arizona • 5/85 to current	• 8-hour and 24-hour samples for 0-2.5, 0-10, and 0-15 µm size ranges and analyzed for mass, elements, ions, and carbon. Meteorological measurements are also available. A major summer intensive study was conducted in summer, 1987, to develop a regional profile for the South Coast Air Basin and to detect contributions from this urban area in the Grand Canyon.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
25. "WHITEX" - Winter Haze Intensive Tracer Experiment (Malm et al., 1989)	• 2 sites in Arizona, 2 sites in Utah, 8 secondary sites (1 in Arizona, 7 in Utah) • 1/87 to 2/87	• 6-hour and 12-hour samples for 0-2.5 μm size ranges. Six DRUM samplers were also operated concurrently to collect 9 particle size ranges between 0.07 and 8.5 μm size ranges. Samples were analyzed for mass, elements, ions, carbon, absorption, and hydrogen. • Chemical mass balance and other receptor modeling techniques will be applied.
26. "IMPROVE" - Interagency Monitoring and Protected Visual Environments (Joseph et al., 1987)	Regional Scale: • 36 sites in United States (20 IMPROVE sites and 16 NPS sites) • 10/87 to 9/90	• 24-hour samples are collected and analyzed for mass, elements, ions, carbon, and hydrogen.
27. "WRAQS" - Western Regional Air Quality Study (Tombach et al., 1987)	Regional Scale: • 10 sites in California, Arizona, Utah, Colorado, Montana, Idaho, New Mexico, and Wyoming • 7/80 to 10/82	• 3-hour, 4-hour, and 8-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass, elements, ions, and carbon.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
28. "WFPS" - Western Fine Particle Study (Flocchini et al., 1981; Cahill et al., 1981)	Regional Scale: • 40 sites in Montana, North Dakota, South Dakota, Wyoming, Utah, New Mexico, Colorado, and Arizona • 10/79 to 5/80	• 72-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass and elements. • Factor analysis was applied to describe the spatial and temporal variations.
29. NPS Particulate Monitoring Network (Cahill et al., 1986)	Regional Scale: • 34 sites in Washington, Oregon, California, Montana, Idaho, North and South Dakota, Colorado, Nevada, Utah, Arizona, N. Mexico, Texas Arkansas, Tennessee, and Virginia • 6/82 to 5/86	• 72-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass, elements, hydrogen, and b_{abs}. • Chemical mass balance was applied on selected sites.
30. Harvard Air Pollution Health Effects Study (Spengler and Thurston, 1984)	Regional Scale: • 6 sites in Massachusetts, Tennessee, Kansas, Wisconsin, Ohio, and Missouri • 2/79 to 7/81	• 24-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass and elements. • Chemical mass balance and principal component analysis were applied.

TABLE 2 (continued)

AMBIENT PARTICULATE DATA BASES

Study and Reference	Site Location and Study Period	Study Description
31. U.S. EPA Inhalable Particulate Matter Network (Watson et al., 1981; Rogers and Watson, 1984)	Urban and Regional Scale: • 73 sites in United States • 5/79 to 6/80	• 24-hour samples for 0-2.5 and 2.5-15 μm size ranges and analyzed for mass elements and ions. • Chemical mass balance was applied on selected sites.

SECTION 7

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APPENDIX A
THEORY OF THE CHEMICAL MASS BALANCE RECEPTOR MODEL

APPENDIX A

THEORY OF THE CHEMICAL MASS BALANCE RECEPTOR MODEL

A.1 INTRODUCTION

Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to the receptor. The particle characteristics must be such that: 1) they are present in different proportions in different source emissions; 2) these proportions remain relatively constant for each source type; and 3) changes in these proportions between source and receptor are negligible or can be approximated.

Common types of receptor models include: 1) chemical mass balance (CMB); 2) principal component analysis (PCA, otherwise known as factor analysis); and 3) multiple linear regression (MLR). Extensive explanations of each of these models, operating separately and together, are given by Watson (1984), Chow (1985), Hopke (1985), and Watson et al. (1987a; 1987b). The PCA, CMB, and MLR have been combined with a dispersion model in a PM_{10} assessment package prepared for the California Air Resources Board (Freeman et al., 1987; Watson et al., 1987a) which provides interfaces among data bases and modeling software. The chemical mass balance (CMB) is the fundamental receptor model, and the derivation of the PCA and MLR models from fundamental physical principles begins with the CMB.

The chemical mass balance consists of a least squares solution to a set of linear equations which expresses each receptor concentration of a chemical species as a linear sum of products of source profile species and source contributions. The source profile species (i.e., the fractional amount of the species in the emissions from each source-type) and the receptor concentrations, with appropriate uncertainty estimates, serve as input data to the CMB model. The output consists of the amount contributed by each source-type to each chemical species. The model calculates values for the contributions from each source and the uncertainties of those values. Input data uncertainties are used both to weight the importance of input data values in the solution and to calculate the uncertainties of the source contributions.

A.2 DERIVATION, EQUATIONS, AND SOLUTIONS

The concentration measured at a receptor during a sampling period of length T due to a source j with constant emission rate E_j is

$$S_j = D_j \cdot E_j \qquad \text{(A-1)}$$

where

$$D_j = \int_0^T d\,[\vec{u}(t), \sigma(t), \vec{x}_j]\,dt \qquad \text{(A-2)}$$

is a dispersion factor depending on wind velocity (u), atmospheric stability (σ), and the location of source j with respect to the receptor (x_j). All parameters in Equation A-2 vary with time, so the instantaneous dispersion factor, d, must be an integral over time period T (Watson, 1979).

Various forms for d have been proposed (Pasquill, 1974; Seinfeld, 1975; Benarie, 1976), some including provisions for chemical reactions, removal, and specialized topography. None are completely adequate to describe the complicated, random nature of dispersion in the atmosphere. The advantage of receptor models is that an exact knowledge of D_j is unnecessary.

If a number of sources, J, exists and there is no interaction between their emissions to cause mass removal, the total mass measured at the receptor, C, will be a linear sum of the contributions from the individual sources.

$$C = \sum_{j=1}^{J} D_j \cdot E_j = \sum_{j=1}^{J} S_j \qquad \text{(A-3)}$$

Similarly, the concentration of elemental component i, C_i will be

$$C_i = \sum_{j=1}^{J} F_{ij} \cdot S_j \qquad i = 1,\ldots I \qquad \text{(A-4)}$$

where F_{ij} = the fraction of source contribution S_j composed of element i.

The number of chemical species (I) must be greater than or equal to the number of sources (J) for a unique solution to these equations.

Solutions to the CMB equations consist of: 1) a tracer solution; 2) a linear programming solution; 3) an ordinary weighted least squares solution with or without an intercept; 4) a ridge regression weighted least squares solution with or without an intercept; and 5) an effective variance least squares solution with or without an intercept. An estimate of the uncertainty associated with the source contributions is an integral part of several of these solution methods.

Weighted linear least squares solutions are preferable to the tracer and linear programming solutions because: 1) theoretically they yield the most likely solution to the CMB equations, providing model assumptions are met; 2) they can make use of all available chemical measurements, not just the so-called tracer species; 3) they are capable of analytically estimating the uncertainty of the source contributions; and 4) there is, in practice, no such thing as a "tracer."

CMB software in current use applies the effective variance solution developed and tested by Watson et al. (1984) because this solution: 1) provides realistic estimates of the uncertainties of the source contributions (owing to its incorporation of both source profile and receptor data uncertainties); and 2) gives greater influence to chemical species with higher precisions in both the source and receptor measurements are than to species with lower precisions.

The effective variance solution is derived by minimizing the weighted sums of the squares of the differences between the measured and calculated values of C_i and F_{ij} (Britt and Luecke, 1973). The solution algorithm is an iterative procedure which calculates a new set of S_j based on the S_j estimated from the previous iteration. It is carried out by the following steps expressed in matrix notation. A superscript k is used to designate the value of a variable at the kth iteration.

1. Set initial estimate of the source contributions equal to zero.

$$S_j^{k=0} = 0 \qquad j=1,..J \tag{A-5}$$

2. Calculate the diagonal components of the effective variance matrix, V_e. All off-diagonal components of this matrix are equal to zero.

$$V_{eii}^{k} = \sigma_{Ci}^{2} + \Sigma(S_j^{k})^{2} \cdot \sigma_{Fij}^{2} \tag{A-6}$$

3. Calculate the k+1 value of S_j

$$S^{k+1} = (F^T (V_e^k)^{-1} F)^{-1} F^T (V_e^k)^{-1} C \tag{A-7}$$

4. Test the (k+1)th iteration of the S_j against the kth iteration. If any one differs by more than 1 percent, then perform the next iteration. If all differ by less than 1 percent, then terminate the algorithm.

$$\text{if} \quad S_j^{k+1} - S_j^{k} / S_j^{k+1} > 0.01 \quad \text{go to step 2}$$

$$\text{if} \quad S_j^{k+1} - S_j^{k} / S_j^{k+1} \leq 0.01 \quad \text{go to step 5} \tag{A-8}$$

5. Assign the (k÷1)th iteration to S_j and σ_{Sj}. All other calculations are performed with these final values.

$$\sigma_{Sj} = [(F^T (V_e^{k+1})^{-1} F)^{-1}_{jj}]^{1/2} \qquad j = 1,..J \tag{A-9}$$

where C = $(C_1 ... C_I)^T$, a column vector with C_i as the ith component

S = $(S_1 ... S_J)^T$, a column vector with S_j as the jth component

F = An I x J matrix of F_{ij}, the source composition matrix

σ_{Ci} = One standard deviation precision of the C_i measurement

σ_{Fij} = One standard deviation precision of the F_{ij} measurement

V_e = Diagonal matrix of effective variances

This effective variance solution algorithm is very general, and it reduces to most of the solutions cited above with the following modifications:

- When the $\sigma_{F_{ij}}$ are set equal to zero, the solution reduces to the ordinary weighted least squares solution.
- When the $\sigma_{F_{ij}}$ are set equal to the same constant value, the solution reduces to the unweighted least squares solution.
- When a column is added to the F_{ij} matrix with all values equal to 1, an intercept term is computed for the variable corresponding to this column.
- When the number of source profiles equals the number of species (I=J), and if the selected species are present only in a single, exclusive source profile, the solution reduces to the tracer solution.
- When the matrix

  $$(F^T (V_e^k)^{-1} F) \tag{A-10}$$

  is re-written as

  $$(F^T (V_e^k)^{-1} F - \varphi I) \tag{A-11}$$

  with φ equal to some non-zero number, known as the smoothing parameter, and I equal to the identity matrix, the solution becomes the ridge regression solution (Williamson and DuBose, 1983).

Watson (1979) found that individual sources with similar source profiles would yield unreliable values if included in the same chemical mass balance. Henry (1982) proposed a quantitative method of identifying this interference between these similar source compositions, which is known as "collinearity." His "singular value decomposition" defines an "estimable space into which resolvable sources should lie." The sources which do not fall into this estimable space are collinear, or too similar to be resolved from the sources which do lie within the estimable space. Henry (1982) further proposed that linear combinations of source contributions resulting from collinear source compositions would be more representative of the summed contributions of these sources.

Williamson and Dubose (1983) claimed that the ridge regression reduces collinearities. Henry (1982) tested the ridge regression solution with respect to the separation of urban and continental dust and found that the bias resulted in physically unrealistic negative values for several of the F_{ij}. The ridge regression solution has not been used in the CMB since these tests were published.

Formulas for the performance measures are:

$$\text{Reduced chi square} = X^2 = \frac{1}{I-J} \sum_{i=1}^{I} [(C_i - \sum_{j=1}^{J} F_{ij}S_j)^2/V_{eii}] \tag{A-12}$$

$$\text{Percent Mass} = 100(\sum_{j=1}^{J} S_j)/C_t,$$ where C_t denotes the total measured mass

$$\text{R square} = 1 - [\,(I-J)X^2]/[\sum_{i=1}^{I} C_i^2/V_{eii}] \tag{A-13}$$

$$\text{Modified Pseudo-Inverse Matrix} = (F^T(V_e)^{-1}F)^{-1}F^T(V_e)^{-1} \tag{A-14}$$

The Singular Value Decomposition of the weighted F matrix is given by

$$V_e^{-\frac{1}{2}}F = UDV^T \tag{A-15}$$

where U and V are IxI and JxJ orthogonal matrices, respectively, and where D is a diagonal matrix with J nonzero and positive elements called the singular values of the decomposition. The columns of V are called the eigenvectors of the composition and their components are associated with source types mentioned earlier in the discussion of the Similarity/Uncertainty Cluster Display.

The maximum size of the CMB7 work array, which determines how many source profiles and fitting species can be used by the software, can be estimated from the following sum:

Work array size (in 4-byte floating point units) =

$$11M + 13I' + 8J' + 2I'J' + 5IJ + 4J \tag{A-16}$$

where

M = number of receptor samples

I' = number of species (fitting and floating)

J' = number of source profiles (fitting and floating)

I = maximum number of fitting species

J = maximum number of fitting sources

The work array size must be less than the number which appears after the introductory banner in CMB7 (see Section 3.2).

A.3 CMB MODEL ASSUMPTIONS

The CMB model assumptions are:

1. Compositions of source emissions are constant over the period of ambient and source sampling.
2. Chemical species do not react with each other, i.e., they add linearly.
3. All sources with a potential for significantly contributing to the receptor have been identified and have had their emissions characterized.
4. The source compositions are linearly independent of each other.
5. The number of sources or source categories is less than or equal to the number of chemical species.
6. Measurement uncertainties are random, uncorrelated, and normally distributed.

A.4 EFFECTS OF DEVIATIONS FROM CMB MODEL ASSUMPTIONS

Assumptions 1 through 6 for the CMB model are fairly restrictive and will never be totally complied with in actual practice. Fortunately, the CMB model can tolerate deviations from these assumptions, though these deviations increase the stated uncertainties of the source contribution estimates.

The CMB model has been subjected to a number of tests to determine its abilities to tolerate deviations from model assumptions (Watson, 1979; Gordon et al., 1981; Henry, 1982; Currie et al., 1984; Dzubay et al., 1984; Watson and Robinson, 1984; DeCesar et al., 1985; Javitz et al.,1988a, 1988b; and Watson et al., 1987b). These studies all point to the same basic conclusions regarding deviations from the above-stated assumptions.

With regard to Assumption 1, source compositions, as seen at the receptor, are known to vary substantially among sources, and even within a single source over an extended period of time. These variations are both systematic and random and are caused by three phenomena: 1) transformation and deposition between the emissions point and the receptor; 2) differences in fuel type and operating processes between similar sources or the same source in time; and 3) uncertainties or differences between the source profile measurement methods. Evaluation studies have generally compared CMB results from several tests using randomly perturbed input data and from substitutions of different source profiles for the same source type. The general conclusions drawn from these tests are as follows:

- The error in the estimated source contributions due to biases in all of the elements of a source profile is in direct proportion to the magnitude of the biases.
- For random errors, the magnitude of the source contribution errors decreases as the difference between the number of species and sources increases.

The most recent and systematic tests are those of Javitz et al. (1988b) which apply to a simple 4-source urban airshed and a complex 10-source urban airshed. These tests with 17 commonly measured chemical species showed that primary mobile, geological, coal-fired power plant, and vegetative burning source-types can be apportioned with uncertainties of approximately 30% when coefficients of variation in the source profiles are as high as 50%. This performance was demonstrated even without the presence of unique "tracer" species such as selenium for coal-fired power plants or soluble potassium for vegetative burning. In a complex urban airshed, which added residual oil combustion, marine aerosol, steel production, lead smelting, municipal incineration, and a continental background aerosol, it was found that the geological, coal-fired power plant, and background source profiles were collinear with the measured species. At coefficients of variation in the source profiles as low as 25%, average absolute errors were on the order of

60%, 50%, and 130% for the geological, coal-burning, and background sources, respectively. All other sources were apportioned with average absolute errors of approximately 30% even when coefficients of variation in the source profiles reached 50%. Once again, these tests were performed with commonly measured chemical species, and results would improve with a greater number of species which are uniquely emitted by the different source types.

With regard to the nonlinear summation of species, Assumption 2, no studies have been performed to evaluate deviations from this assumption. While these deviations are generally assumed to be small, conversion of gases to particles and reactions between particles are not inherently linear processes. This assumption is especially applicable to the end products of photochemical reactions and their apportionment to the sources of the precursors. Further model evaluation is necessary to determine the tolerance of the CMB model to deviations from this assumption. The current practice is to apportion the primary material which has not changed between source and receptor. The remaining quantities of reactive species such as ammonium, nitrate, sulfate, and elemental carbon are then apportioned to chemical compounds rather than directly to sources. While this approach is not as satisfying as a direct apportionment, it at least separates primary from secondary emitters and the types of compounds apportioned give some insight into the chemical pathways which formed them. As chemical reaction mechanisms and rates, deposition velocities, atmospheric equilibrium, and methods to estimate transport and aging time become better developed, it may be possible to produce "fractionated" source profiles which will allow this direct attribution of reactive species to sources. Such apportionment will require measurements of gaseous as well as particulate species at receptor sites.

A major challenge to the application of the CMB is the identification of the primary contributing sources for inclusion in the model, Assumption 3. Watson (1979) systematically increased the number of sources contributing to his simulated data from four to eight contributors while solving the CMB equations assuming only four sources. He also included more sources in the least squares solutions than those which were actually contributors, with the following results:

- Underestimating the number of sources had little effect on the calculated source contributions if the prominent species contributed by the missing sources were excluded from the solution.

- When the number of sources was underestimated, and when prominent species of the omitted sources were included in the calculation of source contributions, the contributions of sources with properties in common with the omitted sources were overestimated.

- When source-types actually present were excluded from the solution, ratios of calculated to measured concentrations were often outside of the 0.5 to 2.0 range, and the sum of the source contributions was much less than the total measured mass. The low calculated/measured ratios indicated which source compositions should be included.

- When the number of sources was overestimated, the sources not actually present yielded contributions less than their standard errors if their source profiles were significantly distinct from those of other sources. The over-specification of sources decreased the standard errors of the source contribution estimates.

Recent research suggests that Assumption 3 should be restated to specify that source contributions above detection limits should be included in the CMB. At this time, however, it is not yet possible to determine the "detection limit" of a source contribution at a receptor since this is a complicated and unknown function of the other source contributions, the source composition uncertainties and the uncertainties of the receptor measurements. Additional model testing is needed to define this "detection limit."

The linear independence of source compositions required by Assumption 4 has become a subject of considerable interest since the publication of Henry's (1982) singular value decomposition (SVD) analysis. As previously noted, this analysis provides quantitative measures of collinearity and the sensitivity of CMB results to specific receptor concentrations. These measures can be calculated analytically in each application. Henry (1982) also proposed an optimal linear combination of source contributions that have been determined to be collinear.

Other "regression diagnostics" have been summarized by Belsley et al. (1980) and have been applied to the CMB by DeCesar et al. (1985a, 1985b). Kim and Henry (1989) show that most of these diagnostics are useless because they are based on the assumption of zero uncertainty in the source profiles. Kim and Henry demonstrate, through the examination of randomly perturbed model input data, that the values for these diagnostics vary substantially with typical random changes in the source profiles.

Tests performed on simulated data with obviously collinear source compositions typically result in positive and negative values for the collinear source types as well as large standard errors in the collinear source contribution estimates. Unless the source compositions are nearly identical, the sum of these large positive and negative values very closely approximates the sum of the true contributions.

With most commonly measured species (e.g., ions, elements, and carbon) and source-types (e.g., motor vehicle, geological, residual oil, sea salt, steel production, wood burning, and various industrial processes), from five to seven sources are linearly independent of each other in most cases (Javitz et al., 1988b).

Gordon et al. (1981) found instabilities in the ordinary weighted least square solutions to the CMB equations when species presumed to be "unique" to a certain source type were removed from the solution. Using simulated data with known perturbations ranging from 0 to 20%, Watson (1979) found: "In the presence of likely uncertainties, sources such as urban dust and continental background dust cannot be adequately resolved by least squares fitting, even though their compositions are not identical. Several nearly unique ratios must exist for good separation."

With regard to Assumption 5, the true number of individual sources contributing to receptor concentrations is generally much larger than the number of species that can be measured. It is therefore necessary to group sources into source-types of similar compositions so that this assumption is met. For the most commonly measured species, meeting Assumption 4 practically defines these groupings.

With respect to Assumption 6 (the randomness, normality, and the uncorrelated nature of measurement uncertainties), there are no results available from verification or evaluation studies. Every least squares solution to the CMB equations requires this assumption, as demonstrated by the derivation of Watson et al. (1984). In reality, very little is known about the distribution of errors for the source compositions and the ambient concentrations. If anything, the distribution probably follows a log-normal rather than a normal distribution. Ambient concentrations can never be negative, and a normal distribution allows a substantial proportion of negative values, while a log-normal distribution allows no negative values. For small errors (e.g., less than 20%), the actual distribution may not be important, but for large errors it probably is important. A symmetric distribution becomes less probable as the coefficient of variation of the measurement increases. This is one of the most important assumptions of the solution method that requires testing.

A.5 MODEL INPUT AND OUTPUT DATA

The chemical mass balance modeling procedure requires: 1) identification of the contributing sources-types; 2) selection of chemical species to be included; 3) estimation of the fraction of each of the chemical species which is contained in each source- type (i.e., the source compositions); 4) estimation of the uncertainty in both ambient concentrations and source compositions; 5) solution of the chemical mass balance equations, and 6) validation and reconciliation. Each of these steps requires different types of data.

Emissions inventories are examined to determine the types of sources which are most likely to influence a receptor. Principal components analysis applied to a time series of chemical measurements is also a useful method of determining the number and types of sources. After these sources have been identified, profiles acquired from similar sources (Chow and Watson, 1989, identify most of the available source profiles) are examined to select the chemical species to be measured. Watson (1979) demonstrates that the more species measured, the better the precision of the CMB apportionment.

The ambient concentrations of these species, C_i, and their fractional amount in each source-type emission, F_{ij}, are the measured quantities which serve as CMB model input data. These values require uncertainty estimates, σ_{Ci} and σ_{Fij}, which are also input data. Input data uncertainties are used both to weight the importance of input data values in the solution and to calculate the uncertainties of the source contributions. The output consists of: 1) the source contribution estimates (S_j) of each source-type; 2) the standard errors of these source contribution estimates; and 3) the amount contributed by each source-type to each chemical species.

APPENDIX B
CMB7 ERROR MESSAGES AND CORRECTIVE ACTION

APPENDIX B

CMB7 ERROR MESSAGES AND CORRECTIVE ACTION

CMB7 will provide error messages which indicate the corrective actions which must be taken to eliminate the difficulty. Following is a list of the most common error messages, their most probable cause, and the actions which might be taken to correct them.

File system error in file CMBOUT Error Code 1034, Status 004

This error occurs when the number of files in the CONFIG.SYS file located in the root directory is less than 14. Edit this file to contain the line FILES=14, then re-boot the system.

Error opening (XXXXXX.XXX) What is the name of your ______________

This error occurs when a file name given to the program does not exist or is indirect, when the filename extender has not been properly specified, or when the CONFIG.SYS file has specified files less than 14. Verifying and correcting the input files names in the INXXXXXX.IN7 file will usually solve this problem.

AKT*JEFFIN*AK MATRIX IN SUB-ROUTINE CEB2 NEEDS IMPROVEMENT

This error message is given when a matrix cannot be inverted. This can happen when the number of fitting sources exceeds the number of fitting species or when one or more of the profiles have zero values for all of the fitting species. The problem can be solved by reducing the number of fitting sources or by increasing the number of fitting species.

**Some receptor concentration standard errors are less than or equal to zero. Weighted regression cannot be done in this case or
FITTING ELEMENT # XX HAS NON-POSITIVE UNCERTAINTY - .00000 PLEASE REPLACE WITH POSITIVE DETECTION LIMIT PROGRAM TERMINATED Stop- Program terminated.**

Preceding page blank

CMB7 forces the user to assign uncertainties to his input data. Examine the input data files to assure that all receptor concentrations have been assigned non-zero and non-negative precisions. Edit the files to correct them.

No receptor site selected

No samples have been selected by Command 3. Invoke command 3 and examine the choices. Selected samples are followed by a '*'.

File not found in file _________ Error Code 1032, Status 000A

The proper filename extension has not been used in the input file names. Edit the files such that data files have the .TXT extender for CMB7 or the .DAT extender for CMB 6.0 files.

RECORD NUMBER XX OF SOURCE (or POLLUTANT) NAME FILE XXXXXX>XXX DID NOT MATCH THE REQUIRED FORMAT (I2, 2X, A8, A1) AND WAS IGNORED or RECORD NUMBER XXX OF SOURCE COMPOSITION FILE XXXXXX.XXX DID NOT MATCH THE REQUIRED FORMAT AND WAS IGNORED

The input data record is improperly formatted. Examine the input data file and correct the formatting error in a text editor. If the second error prompt is given, the CMB may run, but it may give erroneous values. The source composition data should be verified using Command 11.

AN UNIDENTIFIED POLLUTANT CODE # XX WAS FOUND IN FILE XXXXXX>XXX SOURCE -SO4

A pollutant code found in the source composition file did not appear in the pollutant name file using CMB 6.0 formats. The model will ignore this species.

********** in any output field**

The results of the model exceed the limitations of the output formats. The number is usually meaningless when this appears.

No convergence after 20 iterations - ENTER a carriage return to VIEW RESULTS

This message is given when the effective variance solution has not converged on a set of source contribution estimates. It is usually associated with collinear profiles. Change profiles to obtain convergence.

APPENDIX C

PRINTOUT OF TEST DATA FOR PACS1

```
C>CD CMB
C>CMB7
MAKE SURE THAT YOUR CAPS LOCK IS ON ! ! !


DISK FILE FOR INITIAL INPUT?
IF NOT ENTER CARRIAGE RETURN
IF SO ENTER NAME OF DISK FILE

DO YOU WISH TO RENAME CMBOUT?
IF NOT ENTER A CARRIAGE RETURN.
IF SO ENTER THE FILE NAME.

****************************************************************************
*                                                                          *
*              U. S. EPA CHEMICAL MASS BALANCE RECEPTOR MODEL              *
*                      *** IBM-PC  CMB7  89338 ***                         *
*                                                                          *
*      EPA PROJECT MGRS: THOMPSON G. PACE III, PE                          *
*                        QUANG NGUYEN                                      *
*                        U.S. ENVIRONMENTAL PROTECTION AGENCY              *
*                        OFFICE OF AIR QUALITY PLANNING AND STANDARDS      *
*                        RESEARCH TRIANGLE PARK, NC                        *
*                        (919)-541-5585                                    *
*                                                                          *
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*     MR. QUANG NGUYEN                                                     *
****************************************************************************
     77540

Initialize size fraction by selecting receptor site
Strike enter to continue
   1 PACS1         08/13/77 24 0  COARS
   2 PACS1         08/13/77 24 0  FINE
   3 PACS2         01/24/78 24 0  COARS
   4 PACS2         01/24/78 24 0  FINE
   5 PACS3         08/07/77 24 0  COARS
   6 PACS3         08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 1

   1 PACS1         08/13/77 24 0  COARS *
   2 PACS1         08/13/77 24 0  FINE
   3 PACS2         01/24/78 24 0  COARS
   4 PACS2         01/24/78 24 0  FINE
   5 PACS3         08/07/77 24 0  COARS
   6 PACS3         08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 2

   1 PACS1         08/13/77 24 0  COARS *
   2 PACS1         08/13/77 24 0  FINE  *
   3 PACS2         01/24/78 24 0  COARS
   4 PACS2         01/24/78 24 0  FINE
   5 PACS3         08/07/77 24 0  COARS
   6 PACS3         08/07/77 24 0  FINE

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu:  <ENTER>
```

Preceding page blank

```
 1 Change Fitting Species
 2 Change Fitting Sources
 3 Select Samples
 4 Advance to Next Sample
 5 Calculate Source Contributions
 6 Perform Autofit
 7 Present Data
 8 Present Source Contributions
 9 Write CMB Information to Disk
10 Present Computed Averages of CMB Series
11 Present Source Profile or Receptor Concentrations
12 Write Source Contributions to Species to Disk
13 Graph
14 Present Normalized (over species) MPIN Matrix
15 Exit

Type the line number to select: 5

SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1           DATE: 08/13/77    CMB7  89338
SAMPLE DURATION        24     START HOUR          0           SIZE:    COARS
      R SQUARE        .97    PERCENT MASS     100.6
    CHI SQUARE       1.44              DF        13

  SOURCE
     * TYPE      SCE(UG/M3)     STD ERR       TSTAT
-------------------------------------------------
1       MARIN      10.6029       1.8240      5.8131
3       UDUST       9.5985       1.2616      7.6081
4       AUTPB       9.0906       1.3961      6.5112
5       RDOIL       9.7127       1.6108      6.0296
8       KRAFT      12.3265       7.9102      1.5583
11      ALPRO      11.0997       2.2441      4.9462
12      STEEL       8.1587       1.5239      5.3538
13      FERMN       9.8720       1.6165      6.1072
-------------------------------------------------

MEASURED CONCENTRATION FINE/COARSE/TOTAL:
     80.0+-    8.0/     80.0+-     8.0/     160.0+-    11.3
Strike enter to continue

       UNCERTAINTY/SIMILARITY CLUSTERS        CMB7  89338     SUM OF CLUSTER SOURCES
-------------------------------------------------------------------------------------
-------------------------------------------------------------------------------------
Strike enter to continue
-------------------------------------------------------------------------------------

SPECIES CONCENTRATIONS -  SITE: PACS1          DATE: 08/13/77       CMB7  89338
SAMPLE DURATION        24       START HOUR          0         SIZE:     COARS
      R SQUARE        .97     PERCENT MASS      100.6
    CHI SQUARE       1.44               DF         13

SPECIES-------I---MEAS-------------------CALC-------------RATIO C/M----RATIO R/U
C1     TOT   T  80.00000+-   8.00000  80.46161+-   6.36458   1.01+-  .13     .0
C9     F           .73400+-   .07300    .50073+-    .22362    .68+-  .31   -1.0
C11    NA    *    6.33000+-   .63300   6.07759+-    .47089    .96+-  .12    -.3
C12    MG    *    1.48000+-   .14800   1.48676+-    .52389   1.00+-  .37     .0
C13    AL    *    4.84000+-   .48400   4.40992+-    .55081    .91+-  .15    -.6
C14    SI    *    3.27000+-   .32700   3.38783+-    .15779   1.04+-  .11     .3
C16    S          2.50000+-   .25000   2.41256+-    .28216    .97+-  .15    -.2
C17    CL    *    4.67000+-   .46700   5.19693+-   1.07658   1.11+-  .26     .4
C19    K     *    1.12000+-   .11200   1.44197+-    .38620   1.29+-  .37     .8
C20    CA    *    1.52000+-   .15200   1.47195+-    .10333    .97+-  .12    -.3
C22    TI    *     .14000+-   .01400    .13692+-    .03204    .98+-  .25    -.1
C23    V     *     .27700+-   .02800    .34841+-    .07289   1.26+-  .29     .9
C24    CR    *     .00800+-   .00100    .24531+-    .11640  30.66+-15.05    2.0
C25    MN    *    2.47000+-   .24700   2.43813+-    .12229    .99+-  .11    -.1
C26    FE    *    5.41000+-   .54100   4.11644+-    .30571    .76+-  .09   -2.1
C28    NI    *     .77900+-   .07800    .63016+-    .11802    .81+-  .17   -1.1
C29    CU    *     .05000+-   .00500    .06613+-    .00683   1.32+-  .19    1.9
C30    ZN    *     .21400+-   .02100    .23739+-    .03413   1.11+-  .19     .6
```

```
Strike enter to continue

C35    BR    *    .52000+-   .05200    .51378+-   .15795    .99+-  .32    -.0
C82    PB    *   1.78000+-   .17800   1.93077+-   .27347   1.08+-  .19     .5
C201   OC    *  10.10000+-  1.01000   8.38185+-  1.29686    .83+-  .15   -1.0
C202   EC    *   1.68000+-   .16800   1.34287+-   .39741    .80+-  .25    -.8
C203   SO4   *   8.10000+-   .81300   8.11920+-  1.25659   1.00+-  .18     .0
C204   NO3   *   1.13000+-   .11300    .71048+-   .41362    .63+-  .37   -1.0
--------------------------------------------------------------------------------
Strike enter to continue

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 1

               Sizes:  FINE  COARS
    1 C1       TOT      T     T
    2 C9       F
    3 C11      NA       *     *
    4 C12      MG       *     *
    5 C13      AL       *     *
    6 C14      SI       *     *
    7 C16      S
    8 C17.     CL       *     *
    9 C19      K        *     *
   10 C20      CA       *     *
   11 C22      TI       *     *
   12 C23      V        *     *
   13 C24      CR       *     *
   14 C25      MN       *     *
   15 C26      FE       *     *
   16 C28      NI       *     *
   17 C29      CU       *     *
   18 C30      ZN       *     *
   19 C35      BR       *     *
   20 C82      PB       *     *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: U

               Sizes:  FINE  COARS
    5 C13      AL       *     *
    6 C14      SI       *     *
    7 C16      S
    8 C17      CL       *     *
    9 C19      K        *     *
   10 C20      CA       *     *
   11 C22      TI       *     *
   12 C23      V        *     *
   13 C24      CR       *     *
   14 C25      MN       *     *
   15 C26      FE       *     *
   16 C28      NI       *     *
   17 C29      CU       *     *
   18 C30      ZN       *     *
   19 C35      BR       *     *
   20 C82     PB        *     *
   21 C201    OC        *     *
   22 C202    EC        *     *
   23 C203    SO4       *     *
   24 C204    NO3       *     *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 8

              Sizes:  FINE  COARS
    5 C13     AL        *     *
    6 C14     SI        *     *
    7 C16     S
    8 C17     CL        *
    9 C19     K         *     *
   10 C20     CA        *     *
   11 C22     TI        *     *
   12 C23     V         *     *
   13 C24     CR        *     *
   14 C25     MN        *     *
   15 C26     FE        *     *
   16 C28     NI        *     *
   17 C29     CU        *     *
   18 C30     ZN        *     *
   19 C35     BR        *     *
   20 C82     PB        *     *
   21 C201    OC        *     *
   22 C202    EC        *     *
   23 C203    SO4       *     *
   24 C204    NO3       *     *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu:  <ENTER>

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

Type the line number to select: 2

              Sizes:  FINE  COARS
    1 1       MARIN     *     *
    2 2       CDUST
    3 3       UDUST     *     *
    4 4       AUTPB     *     *
    5 5       RDOIL     *     *
    6 6       VBRN1
    7 7       VBRN2
    8 8       KRAFT     *     *
    9 9       SULFT
   10 10      HOGFU
   11 11      ALPRO     *     *
   12 12      STEEL     *     *
   13 13      FERMN     *     *
   14 14      CARBO
   15 15      GLASS
   16 16      CARBF
   17 17      SO4
   18 18      NO3
```

```
  19 19     OC
  20 20     EC

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 8

            Sizes:  FINE  COARS
   1 1      MARIN    *     *
   2 2      CDUST
   3 3      UDUST    *     *
   4 4      AUTPB    *     *
   5 5      RDOIL    *     *
   6 6      VBRN1
   7 7      VBRN2
   8 8      KRAFT    *
   9 9      SULFT
  10 10     HOGFU
  11 11     ALPRO    *     *
  12 12     STEEL    *     *
  13 13     FERMN    *     *
  14 14     CARBO
  15 15     GLASS
  16 16     CARBF
  17 17     SO4
  18 18     NO3
  19 19     OC
  20 20     EC

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: <ENTER>

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select: 5

NO CONVERGENCE AFTER  20 ITERATIONS.  ENTER A CARRIAGE RETURN TO VIEW RESULTS

SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1       DATE: 08/13/77       CMB7  89338
SAMPLE DURATION        24      START HOUR        0         SIZE:    COARS
       R SQUARE        .90   PERCENT MASS       95.3
     CHI SQUARE      4.46              DF        13

  SOURCE
     * TYPE     SCE(UG/M3)    STD ERR      TSTAT
------------------------------------------------
1      MARIN      12.8176     2.0932     6.1235
3      UDUST      11.7520     1.2217     9.6198
4      AUTPB      10.9940     1.4994     7.3321
5      RDOIL      12.6953     1.8275     6.9467
11     ALPRO      13.5183     2.4576     5.5006
12     STEEL       -.3365      .3005    -1.1196
13     FERMN      14.8274     1.5623     9.4909
------------------------------------------------

MEASURED CONCENTRATION FINE/COARSE/TOTAL:
      80.0+-     8.0/      80.0+-     8.0/     160.0+-    11.3
Strike enter to continue
```

```
       UNCERTAINTY/SIMILARITY CLUSTERS      CMB7  89338   SUM OF CLUSTER SOURCES
----------------------------------------------------------------------------------

----------------------------------------------------------------------------------
Strike enter to continue

SPECIES CONCENTRATIONS -  SITE: PACS1          DATE: 08/13/77      CMB7  89338
SAMPLE DURATION        24       START HOUR         0           SIZE:     COARS
       R SQUARE       .90    PERCENT MASS       95.3
     CHI SQUARE      4.46               DF        13

SPECIES-------I---MEAS-----------------CALC------------RATIO C/M----RATIO R/U
C1      TOT   T  80.00000+-   8.00000  76.26823+-   3.64371     .95+-   .11     -.4
C9      F           .73400+-    .07300    .61844+-    .25714     .84+-   .36     -.4
C11     NA    *    6.33000+-    .63300   6.55688+-    .56405    1.04+-   .14      .3
C12     MG    *    1.48000+-    .14800   1.13935+-    .72038     .77+-   .49     -.5
C13     AL    *    4.84000+-    .48400   5.28780+-    .67072    1.09+-   .18      .5
C14     SI    *    3.27000+-    .32700   3.64568+-    .19486    1.11+-   .13     1.0
C16     S          2.50000+-    .25000   2.40091+-    .35376     .96+-   .17     -.2
C17     CL         4.67000+-    .46700   5.67512+-   1.28691    1.22+-   .30      .7
C19     K     *    1.12000+-    .11200   1.89774+-    .57918    1.69+-   .54     1.3
C20     CA    *    1.52000+-    .15200   1.15141+-    .11617     .76+-   .11    -1.9
C22     TI    *     .14000+-    .01400    .14908+-    .02497    1.06+-   .21      .3
C23     V     *     .27700+-    .02800    .44866+-    .09527    1.62+-   .38     1.7
C24     CR    *     .00800+-    .00100    .01258+-    .00609    1.57+-   .79      .7
C25     MN    *    2.47000+-    .24700   2.55346+-    .14687    1.03+-   .12      .3
C26     FE    *    5.41000+-    .54100   1.53639+-    .24186     .28+-   .05    -6.5
C28     NI    *     .77900+-    .07800    .70895+-    .15383     .91+-   .22     -.4
C29     CU    *     .05000+-    .00500    .04439+-    .00725     .89+-   .17     -.6
C30     ZN    *     .21400+-    .02100    .18537+-    .04604     .87+-   .23     -.6
Strike enter to continue

C35     BR    *     .52000+-    .05200    .61787+-    .19177    1.19+-   .39      .5
C82     PB    *    1.78000+-    .17800   2.26036+-    .33068    1.27+-   .23     1.3
C201    OC    *   10.10000+-   1.01000   8.11265+-   1.39010     .80+-   .16    -1.2
C202    EC    *    1.68000+-    .16800   1.43219+-    .41766     .85+-   .26     -.6
C203    SO4   *    8.10000+-    .81300   8.38399+-   1.60400    1.04+-   .22      .2
C204    NO3   *    1.13000+-    .11300   1.03008+-    .49969     .91+-   .45     -.2
----------------------------------------------------------------------------------
Strike enter to continue

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select: 1

              Sizes:  FINE  COARS
   1 C1       TOT      T      T
   2 C9       F
   3 C11      NA       *      *
   4 C12      MG       *      *
   5 C13      AL       *      *
   6 C14      SI       *      *
   7 C16      S
   8 C17      CL       *
   9 C19      K        *      *
  10 C20      CA       *      *
  11 C22      TI       *      *
```

```
   12 C23     V         *     *
   13 C24     CR        *     *
   14 C25     MN        *     *
   15 C26     FE        *     *
   16 C28     NI        *     *
   17 C29     CU        *     *
   18 C30     ZN        *     *
   19 C35     BR        *     *
   20 C82     PB        *     *

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 8

            Sizes:  FINE  COARS
   1 C1     TOT      T     T
   2 C9     F
   3 C11    NA       *     *
   4 C12    MG       *     *
   5 C13    AL       *     *
   6 C14    SI       *     *
   7 C16    S
   8 C17    CL       *     *
   9 C19    K        *     *
  10 C20    CA       *     *
  11 C22    TI       *     *
  12 C23    V        *     *
  13 C24    CR       *     *
  14 C25    MN       *     *
  15 C26    FE       *     *
  16 C28    NI       *     *
  17 C29    CU       *     *
  18 C30    ZN       *     *
  19 C35    BR       *     *
  20 C82    PB       *     *

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu:  <ENTER>

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

 Type the line number to select: 2

            Sizes:  FINE  COARS
   1 1      MARIN    *     *
   2 2      CDUST
   3 3      UDUST    *     *
   4 4      AUTPB    *     *
   5 5      RDOIL    *     *
   6 6      VBRN1
   7 7      VBRN2
   8 8      KRAFT    *
   9 9      SULFT     *
  10 10     HOGFU
  11 11     ALPRO    *     *
  12 12     STEEL    *     *
  13 13     FERMN    *     *
  14 14     CARBO
```

```
   15 15     GLASS
   16 16     CARBF
   17 17     S04
   18 18     NO3
   19 19     OC
   20 20     EC

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 8

             Sizes:  FINE  COARS
    1 1      MARIN     *     *
    2 2      CDUST
    3 3      UDUST     *     *
    4 4      AUTPB     *     *
    5 5      RDOIL     *     *
    6 6      VBRN1
    7 7      VBRN2
    8 8      KRAFT     *     *
    9 9      SULFT
   10 10     HOGFU
   11 11     ALPRO     *     *
   12 12     STEEL     *     *
   13 13     FERMN     *     *
   14 14     CARBO
   15 15     GLASS
   16 16     CARBF
   17 17     S04
   18 18     NO3
   19 19     OC
   20 20     EC

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu:

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 9

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 12
```

```
    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 4

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 5

 SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1       DATE: 08/13/77      CMB7  89338
 SAMPLE DURATION          24      START HOUR        0           SIZE:     FINE
       R SQUARE          .98    PERCENT MASS      98.7
     CHI SQUARE         1.12              DF        13

   SOURCE
      * TYPE      SCE(UG/M3)     STD ERR      TSTAT
 --------------------------------------------------
 1      MARIN       12.3889      2.2457     5.5167
 3      UDUST        9.5917      1.3876     6.9127
 4      AUTPB       10.0835      1.4942     6.7486
 5      RDOIL       11.0603      1.9239     5.7490
 8      KRAFT        4.6896      5.0467      .9292
 11     ALPRO       10.6023      3.5896     2.9536
 12     STEEL        8.6729      1.3771     6.2979
 13     FERMN       11.8754      1.8321     6.4820
 --------------------------------------------------

 MEASURED CONCENTRATION FINE/COARSE/TOTAL:
      80.0+-     8.0/      80.0+-     8.0/     160.0+-     11.3
 Strike enter to continue

       UNCERTAINTY/SIMILARITY CLUSTERS     CMB7  89338   SUM OF CLUSTER SOURCES
 ------------------------------------------------------------------------------
        1      8                                           17.078+-     4.241
        1      5      8                                    28.139+-     3.833
 ------------------------------------------------------------------------------

 Strike enter to continue

 SPECIES CONCENTRATIONS -  SITE: PACS1       DATE: 08/13/77      CMB7  89338
 SAMPLE DURATION          24      START HOUR        0           SIZE:     FINE
       R SQUARE          .98    PERCENT MASS      98.7
     CHI SQUARE         1.12              DF        13
```

```
SPECIES-------I---MEAS------------------CALC-------------RATIO C/M----RATIO R/U
C1      TOT    T  80.00000+-   8.00000  78.96461+-   4.82449     .99+-  .12    -.1
C9      F           .88300+-    .08800    .67644+-    .24792     .77+-  .29    -.8
C11     NA     *   6.93000+-    .69300   6.97025+-    .56446    1.01+-  .13     .0
C12     MG     *    .43000+-    .04300   1.60951+-    .62627    3.74+- 1.50    1.9
C13     AL     *   4.66000+-    .46600   4.02418+-    .88919     .86+-  .21    -.6
C14     SI     *   3.02000+-    .30200   2.92212+-    .13329     .97+-  .11    -.3
C16     S          2.95000+-    .29500   3.02466+-    .31807    1.03+-  .15     .2
C17     CL     *   5.95000+-    .59500   5.69381+-   1.24836     .96+-  .23    -.2
C19     K      *   1.64000+-    .16400   1.73084+-    .46411    1.06+-  .30     .2
C20     CA     *   1.78000+-    .17800   1.43537+-    .11366     .81+-  .10   -1.6
C22     TI     *    .08300+-    .00800    .10088+-    .01630    1.22+-  .23    1.0
C23     V      *    .37200+-    .03700    .39757+-    .08308    1.07+-  .25     .3
C24     CR     *    .31500+-    .03200    .20976+-    .12151     .67+-  .39    -.8
C25     MN     *   2.99000+-    .29900   2.82844+-    .14115     .95+-  .11    -.5
C26     FE     *   4.53000+-    .45300   4.24446+-    .33269     .94+-  .12    -.5
C28     NI     *    .76500+-    .07700    .68246+-    .13428     .89+-  .20    -.5
C29     CU     *    .04400+-    .00400    .05274+-    .00510    1.20+-  .16    1.3
C30     ZN     *    .22500+-    .02300    .26786+-    .03966    1.19+-  .21     .9

Strike enter to continue

C35     BR     *    .41900+-    .04200    .56133+-    .17386    1.34+-  .44     .8
C82     PB     *   2.53000+-    .25300   2.13749+-    .30300     .84+-  .15   -1.0
C201    OC     *   7.54000+-    .75400   8.50978+-   1.35632    1.13+-  .21     .6
C202    EC     *   1.42000+-    .14200   1.33579+-    .34012     .94+-  .26    -.2
C203    SO4    *  10.30000+-   1.03400   9.78819+-   1.47514     .95+-  .17    -.3
C204    NO3    *    .63800+-    .06400    .88402+-    .35938    1.39+-  .58     .7
-----------------------------------------------------------------------------------

Strike enter to continue

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select: 9

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select: 12
```

```
    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 3

    1 PACS1        08/13/77 24 0  COARS
    2 PACS1        08/13/77 24 0  FINE  *
    3 PACS2        01/24/78 24 0  COARS
    4 PACS2        01/24/78 24 0  FINE
    5 PACS3        08/07/77 24 0  COARS
    6 PACS3        08/07/77 24 0  FINE

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 1

    1 PACS1        08/13/77 24 0  COARS *
    2 PACS1        08/13/77 24 0  FINE  *
    3 PACS2        01/24/78 24 0  COARS
    4 PACS2        01/24/78 24 0  FINE
    5 PACS3        08/07/77 24 0  COARS
    6 PACS3        08/07/77 24 0  FINE

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 2

    1 PACS1        08/13/77 24 0  COARS *
    2 PACS1        08/13/77 24 0  FINE
    3 PACS2        01/24/78 24 0  COARS
    4 PACS2        01/24/78 24 0  FINE
    5 PACS3        08/07/77 24 0  COARS
    6 PACS3        08/07/77 24 0  FINE

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu:

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 5

 SOURCE CONTRIBUTION ESTIMATES -  SITE: PACS1        DATE: 08/13/77     CMB7  89338
 SAMPLE DURATION        24      START HOUR        0        SIZE:    COARS
        R SQUARE       .97    PERCENT MASS    100.6
      CHI SQUARE      1.44              DF       13
```

```
SOURCE
  * TYPE      SCE(UG/M3)   STD ERR      TSTAT
------------------------------------------------
1    MARIN      10.6029     1.8240      5.8131
3    UDUST       9.5985     1.2616      7.6081
4    AUTPB       9.0906     1.3961      6.5112
5    RDOIL       9.7127     1.6108      6.0296
8    KRAFT      12.3265     7.9102      1.5583
11   ALPRO      11.0997     2.2441      4.9462
12   STEEL       8.1587     1.5239      5.3538
13   FERMN       9.8720     1.6165      6.1072
------------------------------------------------

MEASURED CONCENTRATION FINE/COARSE/TOTAL:
     80.0+-     8.0/     80.0+-     8.0/     160.0+-     11.3
Strike enter to continue

       UNCERTAINTY/SIMILARITY CLUSTERS      CMB7  89338  SUM OF CLUSTER SOURCES
-------------------------------------------------------------------------------
-------------------------------------------------------------------------------
Strike enter to continue

SPECIES CONCENTRATIONS -  SITE: PACS1          DATE: 08/13/77
SAMPLE DURATION         24      START HOUR        0                CMB7  89338
       R SQUARE        .97    PERCENT MASS    100.6      SIZE:     COARS
     CHI SQUARE       1.44              DF       13

SPECIES-------I---MEAS------------------CALC-------------RATIO C/M----RATIO R/U
C1     TOT    T  80.00000+-  8.00000  80.46161+-  6.36458   1.01+-  .13      .0
C9     F            .73400+-   .07300    .50073+-   .22362    .68+-  .31    -1.0
C11    NA     *   6.33000+-   .63300   6.07759+-   .47089    .96+-  .12     -.3
C12    MG     *   1.48000+-   .14800   1.48676+-   .52389   1.00+-  .37      .0
C13    AL     *   4.84000+-   .48400   4.40992+-   .55081    .91+-  .15     -.6
C14    SI     *   3.27000+-   .32700   3.38783+-   .15779   1.04+-  .11      .3
C16    S          2.50000+-   .25000   2.41256+-   .28216    .97+-  .15     -.2
C17    CL     *   4.67000+-   .46700   5.19693+-  1.07658   1.11+-  .26      .4
C19    K     .*   1.12000+-   .11200   1.44197+-   .38620   1.29+-  .37      .8
C20    CA     *   1.52000+-   .15200   1.47195+-   .10333    .97+-  .12     -.3
C22    TI     *    .14000+-   .01400    .13692+-   .03204    .98+-  .25     -.1
C23    V      *    .27700+-   .02800    .34841+-   .07289   1.26+-  .29      .9
C24    CR     *    .00800+-   .00100    .24531+-   .11640  30.66+-15.05     2.0
C25    MN     *   2.47000+-   .24700   2.43813+-   .12229    .99+-  .11     -.1
C26    FE     *   5.41000+-   .54100   4.11644+-   .30571    .76+-  .09    -2.1
C28    NI     *    .77900+-   .07800    .63016+-   .11802    .81+-  .17    -1.1
C29    CU     *    .05000+-   .00500    .06613+-   .00683   1.32+-  .19     1.9
C30    ZN     *    .21400+-   .02100    .23739+-   .03413   1.11+-  .19      .6
Strike enter to continue

C35    BR     *    .52000+-   .05200    .51378+-   .15795    .99+-  .32     -.0
C82    PB     *   1.78000+-   .17800   1.93077+-   .27347   1.08+-  .19      .5
C201   OC     *  10.10000+-  1.01000   8.38185+-  1.29686    .83+-  .15    -1.0
C202   EC     *   1.68000+-   .16800   1.34287+-   .39741    .80+-  .25     -.8
C203   SO4    *   8.10000+-   .81300   8.11920+-  1.25659   1.00+-  .18      .0
C204   NO3    *   1.13000+-   .11300    .71048+-   .41362    .63+-  .37    -1.0
-------------------------------------------------------------------------------
Strike enter to continue

 1 Change Fitting Species
 2 Change Fitting Sources
 3 Select Samples
 4 Advance to Next Sample
 5 Calculate Source Contributions
 6 Perform Autofit
 7 Present Data
 8 Present Source Contributions
 9 Write CMB Information to Disk
10 Present Computed Averages of CMB Series
11 Present Source Profile or Receptor Concentrations
12 Write Source Contributions to Species to Disk
13 Graph
```

```
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 11

 WHAT DO YOU WANT TO SEE?
 ENTER S FOR SOURCE PROFILE OR R FOR RECEPTOR CONCENTRATIONS.
 S
 DO YOU WANT TO LOOK AT THE WHOLE MATRIX?
 IT IS 20 SOURCES BY 24 SPECIES
 N
 WHICH SOURCE DO YOU WANT?
 GIVE SOURCE CODE
 4

 SOURCE: AUTPB
 C1      TOT          1.0000   +-     .0000
 C9      F             .0000   +-     .0001
 C11     NA            .0000   +-     .0005
 C12     MG            .0000   +-     .0050
 C13     AL            .0110   +-     .0050
 C14     SI            .0082   +-     .0030
 C16     S             .0040   +-     .0013
 C17     CL            .0300   +-     .0100
 C19     K             .0007   +-     .0003
 C20     CA            .0125   +-     .0050
 C22     TI            .0000   +-     .0010
 C23     V             .0000   +-     .0000
 C24     CR            .0000   +-     .0001
 C25     MN            .0000   +-     .0002
 C26     FE            .0210   +-     .0080
 C28     NI            .0002   +-     .0001
 C29     CU            .0007   +-     .0003
 C30     ZN            .0035   +-     .0013
 C35     BR            .0500   +-     .0170
 C82     PB            .2000   +-     .0300
 C201    OC            .5000   +-     .1000
 C202    EC            .0380   +-     .0140
 C203    SO4           .0130   +-     .0040
 Strike enter to continue

 C204    NO3           .0091   +-     .0030
 Strike enter to continue

 WHICH SOURCE DO YOU WANT?
 GIVE SOURCE CODE

 WHAT DO YOU WANT TO SEE?
 ENTER S FOR SOURCE PROFILE OR R FOR RECEPTOR CONCENTRATIONS.
 OR ARE YOU DONE?
 D

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 8
```

```
                               CALC SPECIES(PER SOURCE)
          INDIVIDUAL RATIO = --------------------------
                               MEAS SPECIES(ALL SOURCES)

                                       SOURCE NAME
    SPECIES   MARIN   UDUST   AUTPB   RDOIL   KRAFT   ALPRO   STEEL   FERMN
     TOT       .133    .120    .114    .121    .154    .139    .102    .123
     F         .000    .001    .000    .007    .000    .635    .000    .039
     NA        .670    .027    .000    .054    .103    .042    .016    .048
     MG        .344    .100    .000    .000    .000    .202    .358    .000
     AL        .000    .131    .021    .011    .007    .718    .011    .013
     SI        .000    .922    .023    .029    .005    .003    .125    .030
     S         .140    .000    .015    .517    .163    .000    .064    .067
     CL        .908    .000    .058    .000    .077    .029    .032    .009
     K         .133    .088    .006    .024    .044    .000    .067    .925
     CA        .098    .189    .075    .101    .029    .059    .333    .084
     TI        .000    .692    .000    .076    .000    .060    .117    .032
     V         .000    .009    .000   1.206    .000    .016    .018    .009
     CR        .000    .540    .000    .571   7.396    .222  21.417    .518
     MN        .000    .004    .000    .002    .003    .000    .287    .691
     FE        .000    .102    .035    .053    .042    .008    .483    .038
     NI        .000    .000    .002    .668    .035    .030    .073    .000
     CU        .000    .058    .133    .146    .148    .311    .457    .071
     ZN        .000    .049    .149    .182    .000    .005    .457    .268
 Strike enter to continue

    SPECIES   MARIN   UDUST   AUTPB   RDOIL   KRAFT   ALPRO   STEEL   FERMN
     BR        .041    .001    .874    .002    .013    .026    .000    .030
     PB        .000    .020   1.021    .006    .000    .000    .035    .002
     OC        .000    .032    .450    .067    .193    .000    .000    .088
     EC        .000    .089    .206    .179    .132    .106    .000    .088
     SO4       .131    .001    .015    .577    .180    .023    .025    .051
     NO3       .000    .002    .073    .056    .000    .000    .000    .498
 Strike enter to continue

     1 Change Fitting Species
     2 Change Fitting Sources
     3 Select Samples
     4 Advance to Next Sample
     5 Calculate Source Contributions
     6 Perform Autofit
     7 Present Data
     8 Present Source Contributions
     9 Write CMB Information to Disk
    10 Present Computed Averages of CMB Series
    11 Present Source Profile or Receptor Concentrations
    12 Write Source Contributions to Species to Disk
    13 Graph
    14 Present Normalized (over species) MPIN Matrix
    15 Exit

 Type the line number to select: 14

                              TRANSPOSE OF SENSITIVITY MATRIX
                                       SOURCE NAME
    SPECIES   MARIN   UDUST   AUTPB   RDOIL   KRAFT   ALPRO   STEEL   FERMN
     NA        1.00     .01    -.05    -.05     .11    -.01    -.10     .03
     MG         .26    -.04     .02    -.00    -.22     .09     .27    -.11
     AL        -.02     .02     .01    -.01    -.18    1.00    -.22     .09
     SI        -.04    1.00    -.02    -.02     .03    -.12    -.19     .04
     CL         .79    -.03     .07    -.02    -.18    -.00     .05    -.05
     K          .00     .07    -.03    -.01     .09     .00    -.29     .52
     CA         .19     .05     .06     .08    -.19     .01     .53    -.14
     TI        -.01     .37    -.02     .05    -.04     .01    -.07     .02
     V          .09    -.03     .06    1.00    -.43     .01    -.07     .01
     CR        -.18    -.06    -.12    -.19     .42    -.08     .28    -.14
     MN        -.03    -.06    -.05    -.04    -.11    -.00    -.02    1.00
     FE        -.03    -.12    -.05    -.10    -.00    -.12    1.00    -.38
     NI         .01    -.04     .00     .79    -.20     .01    -.01    -.03
     CU        -.27    -.12    -.07    -.13     .49     .25     .40    -.16
     ZN         .09    -.11     .14     .19    -.33    -.04     .49     .02
    BR        .10   -.02    .48    .03   -.19    .02   -.03    .01
    PB        .17   -.04   1.00    .09   -.46   -.00    .02   -.05
    OC       -.43    .07    .22   -.25   1.00   -.11   -.39    .14
    EC       -.19    .06    .03    .01    .40    .04   -.22    .10
    SO4      -.17    .01   -.16    .43    .61   -.07   -.28    .07
Strike enter to continue

   SPECIES  MARIN  UDUST  AUTPB  RDOIL  KRAFT  ALPRO  STEEL  FERMN
    NO3      -.01    .02    .03    .04   -.01    .01   -.16    .27
Strike enter to continue

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

 Type the line number to select: 13

    1                   Graph elemental concentrations
    2                              Graph source profiles
    3                         Graph source contributions
    4                                         Graph PM10
    5                                    Exit graph menu

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 1
 Hardcopy?  Y or N
 Y

 Plot file name cmbplot.001
    1                   Graph elemental concentrations
    2                              Graph source profiles
    3                         Graph source contributions
    4                                         Graph PM10
    5                                    Exit graph menu

 Type the line number to select or deselect
 D for page down, U for page up, ENTER for main menu: 2

   1  1      MARIN
   2  2      CDUST
   3  3      UDUST
   4  4      AUTPB
   5  5      RDOIL
   6  6      VBRN1
   7  7      VBRN2
   8  8      KRAFT
   9  9      SULFT
  10  10     HOGFU
  11  11     ALPRO
  12  12     STEEL
  13  13     FERMN
  14  14     CARBO
  15  15     GLASS
  16  16     CARBF
  17  17     SO4
  18  18     NO3
  19  19     OC
  20  20     EC
```

```
Toggle selection, Up or Down, Carriage return to exit: 4

   1  1       MARIN
   2  2       CDUST
   3  3       UDUST
   4  4       AUTPB     *
   5  5       RDOIL
   6  6       VBRN1
   7  7       VBRN2
   8  8       KRAFT
   9  9       SULFT
  10  10      HOGFU
  11  11      ALPRO
  12  12      STEEL
  13  13      FERMN
  14  14      CARBO
  15  15      GLASS
  16  16      CARBF
  17  17      SO4
  18  18      NO3
  19  19      OC
  20  20      EC


Toggle selection, Up or Down, Carriage return to exit:
Hardcopy?  Y or N
N

   1                    Graph elemental concentrations
   2                           Graph source profiles
   3                       Graph source contributions
   4                                      Graph PM10
   5                                  Exit graph menu

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 3
Hardcopy?  Y or N
N

   1                    Graph elemental concentrations
   2                           Graph source profiles
   3                       Graph source contributions
   4                                      Graph PM10
   5                                  Exit graph menu

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu: 5

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select:  6

   1 PACS1        08/13/77 24 0  COARS *
   2 PACS1        08/13/77 24 0  FINE  *
   3 PACS2        01/24/78 24 0  COARS *
   4 PACS2        01/24/78 24 0  FINE  *
   5 PACS3        08/07/77 24 0  COARS *
   6 PACS3       08/07/77 24 0  FINE  *

Type the line number to select or deselect
D for page down, U for page up, ENTER for main menu:

   1 Change Fitting Species
   2 Change Fitting Sources
   3 Select Samples
   4 Advance to Next Sample
   5 Calculate Source Contributions
   6 Perform Autofit
   7 Present Data
   8 Present Source Contributions
   9 Write CMB Information to Disk
  10 Present Computed Averages of CMB Series
  11 Present Source Profile or Receptor Concentrations
  12 Write Source Contributions to Species to Disk
  13 Graph
  14 Present Normalized (over species) MPIN Matrix
  15 Exit

Type the line number to select: 10


OUTPUT WILL GO TO HARDCOPY.
DO YOU WANT IT DISPLAYED AT YOUR TERMINAL INSTEAD?
Y

                                         FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE    (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  MARIN        12.39     10.60     22.99
PACS2         08/07/77  MARIN        -3.42       .31     -3.12
PACS3         08/07/77  MARIN        20.40     15.51     35.91
                                  --------  --------  --------
                         AVERAGE      9.79      8.81     18.60
                     (STD. DEV.)     12.12      7.76     19.88
                                         FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE    (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  UDUST         9.59      9.60     19.19
PACS2         08/07/77  UDUST         1.17     54.03     55.20
PACS3         08/07/77  UDUST        79.18     61.89    141.07
                                  --------  --------  --------
                         AVERAGE     29.98     41.84     71.82
                     (STD. DEV.)     42.82     28.20     62.62
                                         FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE    (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  AUTPB        10.08      9.09     19.17
PACS2         08/07/77  AUTPB        17.07      3.21     20.28
PACS3         08/07/77  AUTPB        23.93     35.26     59.19
                                  --------  --------  --------
                         AVERAGE     17.03     15.85     32.88
                     (STD. DEV.)      6.92     17.06     22.79
                                         FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE    (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  RDOIL        11.06      9.71     20.77
PACS2         08/07/77  RDOIL          .74       .19       .93
PACS3         08/07/77  RDOIL        14.01     12.45     26.46
                                  --------  --------  --------
                         AVERAGE      8.60      7.45     16.06
                     (STD. DEV.)      6.97      6.43     13.40
```

```
                                              FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE     (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  KRAFT         4.69     12.33     17.02
PACS2         08/07/77  KRAFT        14.23       .28     14.51
PACS3         08/07/77  KRAFT        -3.53      9.42      5.89
                                  --------  --------  --------
                         AVERAGE      5.13      7.34     12.47
                      (STD. DEV.)     8.89      6.29      5.84

                                      FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE     (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  ALPRO        10.60     11.10     21.70
PACS2         08/07/77  ALPRO         -.44      4.19      3.75
PACS3         08/07/77  ALPRO        -1.52      4.46      2.94
                                  --------  --------  --------
                         AVERAGE      2.88      6.58      9.46
                      (STD. DEV.)     6.71      3.91     10.61

                                      FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE     (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  STEEL         8.67      8.16     16.83
PACS2         08/07/77  STEEL        -1.00       .56      -.45
PACS3         08/07/77  STEEL         -.02     -2.21     -2.23
                                  --------  --------  --------
                         AVERAGE      2.55      2.17      4.72
                      (STD. DEV.)     5.33      5.37     10.53

                                      FINE     COARS     TOTAL
CMB SITE      DATE      SOURCE     (UG/M3)  (UG/M3)  (UG/M3)
------------  --------  --------  --------  --------  --------

PACS1         01/24/78  FERMN        11.88      9.87     21.75
PACS2         08/07/77  FERMN          .62      -.11       .51
PACS3         08/07/77  FERMN          .09      1.41      1.50
                                  --------  --------  --------
                         AVERAGE      4.20      3.72      7.92
                      (STD. DEV.)     6.66      5.38     11.99
Strike enter to continue

    1 Change Fitting Species
    2 Change Fitting Sources
    3 Select Samples
    4 Advance to Next Sample
    5 Calculate Source Contributions
    6 Perform Autofit
    7 Present Data
    8 Present Source Contributions
    9 Write CMB Information to Disk
   10 Present Computed Averages of CMB Series
   11 Present Source Profile or Receptor Concentrations
   12 Write Source Contributions to Species to Disk
   13 Graph
   14 Present Normalized (over species) MPIN Matrix
   15 Exit

Type the line number to select: 15
C>
```